Book of Abstracts

26th IUPAP Conference of Computational Physics

Oak Ridge National Laboratory
2025

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26th IUPAP Conference of Computational Physics

CCP2025

Book of Abstracts

Contents

Welcome

The IUPAP Conference on Computational Physics is an annual international conference that covers all aspects of computational physics. The conference rotates on a triannual cycle between Europe/Africa, Asia and the Americas. In 2025 the conference is hosted by Oak Ridge National Laboratory in Oak Ridge, Tennessee as a virtual only event.

This conference will highlight advances in applications, algorithms and implementations of computational approaches in all areas of physics.

1. Condensed Matter Physics / Materials
2. Statistical Mechanics
3. Many Body Physics
4. Soft Matter and Polymers
5. Biophysics
6. Fluid Dynamics and Continuum Mechanics
7. Plasma Physics and Fusion
8. Nuclear and Particle Physics
9. Astrophysics, Cosmology and Gravitation
10. Algorithms and Novel Hardware Scientific Computing
11. Applications of Machine Learning and Artificial Intelligence
12. Computational Physics Education

We invite you to register and submit abstracts for oral presentations, posters or tutorials on the conference website: ccp2025.ornl.gov

Registration and attendance of the virtual conference is free.

Deadline for abstract submission: October 26, 2025 Deadline for registration: October 29, 2025

The link for attending the virtual conference will be shared after the registration deadline.

We encourage participation of computational physicists and related disciplines at every career level.

Agenda

All times are Eastern Time (GMT-5).

Time	Monday			Tuesday			Wednesday			Thursday			Friday		
	Plenary	Breakout 1	Breakout 2	Plenary	Breakout 1	Breakout 2	Plenary	Breakout 1	Breakout 2	Plenary	Breakout 1	Breakout 2	Plenary	Breakout 1	Breakout 2
8:00	Welcome				1.15	5.1		1.5	7.1	Poster Session				1.11	1.19
8:10		1.1	1.7												
8:20					1.2	5.3		1.10	8.1					1.17	1.27
8:30		1.13	4.4												
8:40					1.3	5.4		1.31	8.2					1.23	1.33
8:50		1.16	4.1												
9:00					1.6	5.5		11.6	3.3					1.25	1.36
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9:20						5.6		1.8	1.29					1.34	1.35
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9:40					11.4	5.7		11.7	1.28					1.37	2.6
9:50		1.38	4.2												
10:00				Jack Dongarra, University of Tennesse			Angel Rubio, MPI				1.4	2.2		1.41	2.8
10:10		10.2	6.1												
10:20											1.24	2.9		1.42	1.26
10:30	Overview of OLCF														
10:40											1.22	2.4		11.3	2.1
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11:00		10.3	6.2				Brian O'Shea				3.2	2.5		11.8	1.32
11:10															
11:20		2.3	1.30								1.39	2.7		1.18	11.9
11:30															
11:40		3.4	11.5								1.40	10.4	Closing		
11:50															
12:00					1.9	5.2	Markus Buehler, MIT			Felipe Jornada					
12:10															
12:20					12.1	10.1									
12:30															
12:40					11.1	1.12									
12:50															
13:00															

Monday, November 3

Breakout 1

8:10–12:00 Chair: Swarnava Ghosh

8:10 1.1 B. Ujfalussy: Superconducting properties of Fe/Au/Nb heterostructures form first principles

8:30 1.13 K. Palotas: Simulation of scanning tunneling microscopy and spectroscopy from first principles beyond the Tersoff-Hamann approximation

8:50 1.16 S. Bhowmik: Efficient real-space Hubbard-corrected density functional theory (DFT+U) with U from Hybrid functionals

9:10 1.14 M. Eisenbach: Scalable First Principles Calculations for Alloys

9:30 1.21 J. Jakowski: Non-Equilibrium Dynamics of 24,000 Electrons Using Real-Space Multigrids: Implementation, Benchmarking, and Stability

9:50 1.38 S. Das: Large-scale Materials Modeling Using DFT-FE

10:10 10.2 P. Suryanarayana: Real space formalism for hybrid density functionals

10:30 Plenary: Tom Beck: The Oak Ridge Leadership Computing Facility

11:00 10.3 J. Pask: Kohn-Sham calculations from one to a million atoms, from ambient conditions to extreme

11:20 2.3 H. Naguszewski: Comparing the relative efficiency of different parallelisation strategies for Wang-Landau sampling: Case study of high-entropy alloys

11:40 3.4 D. Devore: Applying Tensor Decomposition to Open-Shell CCSD(T)

Breakout 2

8:10–10:10 Chair: Henrik Christiansen

8:10 1.7 M. Dašić: Impact of Water Content on the Mechanical and Thermodynamic Properties of Phosphonium Ionic Liquids

8:30 4.4 J. Payandehpeyman: Micromechanical modeling and numerical evaluation of electrical percolation in carbon nanotube reinforced polymer nanocomposites with homogeneous, agglomerated, and segregated structures

8:50 4.1 M. Severi: Disorder, Dynamics, and Water Confinement in Naphthalene-Diimide Mixed Ionic-Electronic Conductors

9:10 4.5 H. O. Mohammed: Atomistic Origins of Opposite Critical Behavior in Thermoresponsive Ionic Liquid–Water Mixtures: LCST versus UCST

9:30 4.3 M. Ahmed: Investigating the Role of Solvent Quality on the Nonlinear Rheology of Dynamic Covalent Polymer Networks

9:50 4.2 V. Raghuraman: All-Atom Reactive Monte Carlo Molecular Dynamics for Molecular Doping in Organic Semiconductors

10:10 6.1 S. Sinha: The glassy dynamics of multiphase flow: Disorder, frustration and flow regimes

10:30 Plenary: Tom Beck: The Oak Ridge Leadership Computing Facility

11:00–12:00 Chair: Vishnu Raghuraman

11:00 6.2 A. B. Parsa: Analytical Evaluation of Fin Efficiency Using the Homotopy Analysis Method for Fins with Variable Cross-Section and Temperature-Dependent Thermal Conductivity

11:20 1.30 M. Jovanović: Correlation Between Nanoscale Crystallinity, Density, and Hydration in Nafion Membranes: Experimental and Molecular Dynamics Insights

11:40 11.5 H. Christiansen: Fast, Modular, and Differentiable Framework for Machine Learning-Enhanced Molecular Simulations

Tuesday, November 4

Breakout 1

8:00–9:40 Chair: Tanvir Sohail]

8:00 1.15 R Paudel: Semi-Empirical Pseudopotential Method for Low-Dimensional Materials

8:20 1.2 M. Pizzochero: Electrically-tunable ultra-flat bands and π-electron magnetism in graphene nanoribbons

8:40 1.3 G. Fratesi: First-principle simulations of hybrid interfaces: N-heterocyclic carbenes and olefins on metal surfaces and 2D materials

9:00 1.6 T. Sruthi: Engineering Electronic Properties of 2D Materials for Enhanced Supercapacitor Performance

9:20

9:40 11.4 B. Kanungo: Learning local and semi-local density functionals from exact exchange-correlation potentials and energies

10:00 Plenary: Jack Dongarra

11:00

12:00 1.9 S. Singh: Ultralow Lattice Thermal Conductivity and Colossal Thermoelectric Figure of Merit of the Room Temperature Antiferromagnet CsMnBi

12:20 12.1 S. Singh: V2Se2O and Janus V2SeTeO: Monolayer altermagnets for the thermoelectric recovery of low-temperature waste heat

12:40 11.1 V. Baibakova: Programmatic Crystal Structure Generation of Catalyst Materials with AI Agents using Fine-Tuned Large Language Models

Breakout 2

8:00–9:40 Chair: Yuko Okamoto

8:00 5.1 T. P. Duy: Insight of the signal transduction in Adenosine A2A receptor by MD simulations

8:20 5.3 A. Masoumi: Atomistic Molecular Dynamics Determination of the Fundamental Transverse Mode of B-DNA

8:40 5.4 L. V. Phuc: Molecular Dynamic Simulation Study of Deformation Behavior and the Role of Chitosan in Reinforcing Bombyx mori Fibroin Composites Under Acidic Conditions

9:00 5.5 N. V. Gendeshmin: A Fractal Diffusion–Reaction Approach for Modeling Transport and Reactivity in Disordered and Biological Systems

9:20 5.6 Y. Okamoto: Metropolis Monte Carlo Simulations in Amino-Acid Sequence Space of Proteins

9:40 5.7 T. Yamamoto: Simulation of oxygen diffusion in blood flow

10:00 Plenary: Jack Dongarra

11:00

12:00–13:00 Chair: Le Vu Phuc

12:00 5.2 E. Canay: Incorporation of dose-rate effects into the BIANCA biophysical model and application for space radiation risk assessment

12:20 10.1 I. Hen: Permutation matrix representation quantum Monte Carlo: A universal framework for simulating arbitrary quantum many-body systems

12:40 1.12 S. Ray: Investigation of the Proton Transport Mechanism in Sc-Doped CaZrO3 Using Ab-Initio Molecular Dynamics Simulations

Wednesday, November 5

Breakout 1

8:00–9:40 Chair Balazs Ujfalussy

8:00 1.5 J. Jami: Data-driven high-throughput search for the accelerated discovery of rare-earth-free permanent magnets

8:20 1.10 D. Woodgate: Crystallographic orderings in refractory high-entropy superalloys studied via an ab initio concentration wave analysis and atomistic Monte Carlo simulations

8:40 1.31 H. Salahshoor: Deep Learning Solutions for Modeling Microstructure in Materials

9:00 11.6 J. Eller: Machine Learning Excited State Potential Energy Surfaces of Solvated Nile Red with ESTEEM

9:20 1.8 A. Choudhury :Switchable Chern number in van der Waals heterostructures

9:40 11.7 G. Anand: Shannon Entropy-Based Crystal Structure Prediction of Disordered Alloys via Graph Neural Networks with Alchemical Sampling

10:00 Plenary: Angel Rubio: Engineering Quantum Materials via Cavity Vacuum Fluctuations: an ab initio QEDFT framework

11:00 Plenary: Brian W. O'Shea: Simulating magnetized supermassive black hole feedback at the exascale

12:00 Plenary: Markus J. Buehler: Superintelligence for scientific discovery

Breakout 2

8:00–9:40 Chair: Sarah Gregg

8:00 7.1 Y. Nishimura: Two-dimensional and three-dimensional Bohm diffusion in N-body plasma simulation

8:20 8.2 S. Nishimura: Diffusion-model approach to flavor physics: A case study for S4' modular flavor model

8:40 8.2 M. Espain: Commercial CMOS imagers for ionizing radiation detection: morphological analysis for particle classification

9:00 3.3 S. Gregg: Many-body theory of positron binding, annihilation and scattering in molecules

9:20 1.29 Zh. Huang: Vibronic coupling constants calculation with Wannier orbitals for cooperative Jahn-Teller effect

9:40 1.28 N. Tani: SVD-based analysis of time-series data obtained from real-time TDDFT

10:00 Plenary: Angel Rubio: Engineering Quantum Materials via Cavity Vacuum Fluctuations: an ab initio QEDFT framework

11:00 Plenary: Brian W. O'Shea: Simulating magnetized supermassive black hole feedback at the exascale

12:00 Plenary: Markus J. Buehler: Superintelligence for scientific discovery

Thursday, November 6

Breakout 1

8:00 Poster Session

10:00–11:40 Chair: Jaeyun Moon

10:00 1.4 J. Moon: Collective nature of phonon energies beyond harmonic oscillators

10:20 1.24 S. Ghosh: Propagation of elastic waves in a material with strain gradient magnetism

10:40 1.22 I. Vitenburgs: Stochastic Coherent State Path Integral approach to Electrons in a Solid

11:00 3.2 H. Larsson: Rigorously computing thousands of vibrational states using tensor network methods

11:20 1.39 D.-N. Le: vdW-WanMBD: A Wannier-Based DFT Toolkit for calculating van der Waals Interactions

11:40 1.40 D.-N. Le: Quantum Insights into Stick-Slip Phenomena in Nanoscale Tribology

12:00 Plenary: Felipe Jornada

Breakout 2

8:00 Poster Session

10:00–11:40 Chair: Hubert J. Naguszewski

10:00 2.2 L. Shchur: Supervised machine learning of continuous and discontinuous phase transitions

10:20 2.9 W. Janke: Non-universality of aging during phase separation of the two-dimensional long-range Ising model

10:40 2.4 T. Guo: Polynomial-Time Classical Approximate Optimization of Wishart-Planted Spin Glasses

11:00 2.5 S.-H. Tsai: Phase diagram of the square-lattice Potts model in an external field

11:20 2.7 M. Kaur: Machine-Learning Study of Phase Transitions in Ising Models with Competing Interactions

11:40 10.4 D. Gessert: Population annealing in the real microcanonical ensemble

12:00 Plenary: Felipe Jornada

Friday, November 7

Breakout 1

9:00-12:00 Chair: Markus Eisenbach

8:00 1.11 T Kulawardena: Investigation of Piezoelectric Properties of Galfenol - PVDF Interface Using Density Functional Theory

8:20 1.17 M. Sensoy: Transition Metal Doping and Strain as Dual Pathways to Control Adhesion and Conductivity in RuO

8:40 1.23 J. Saha: Distribution of Charge Centers in Matter from Geometric Phases of Electrons

9:00 1.25 B. Das: Competing Electronic, Magnetic, and Volumetric Effects on Hydrogen Binding in Mn/Al Austenitic Iron Alloys

9:20 1.34 N. Mondal: Joint Wannier Centers (JWCs) in Topological insulators: topological transition from the perspective of chemical bonding

9:40 1.37 F. Garadi: Elucidating Nonlinear Optical Behavior in Chalcogenometallates: A DFT Study with Emphasis on Perchalcogenometallates

10:00 1.41 O. Akin-Ojo: Performance of an X-alpha functional in band gap prediction

10:20 1.42 Priyanka: First-Principles Investigation of the Electronic and Vibrational Characteristics of Monolayer WSe2

10:40 11.3 T. Sohail: Bridging Scales with Continuous-Time Neural Operators for History-Dependent Materials

11:00 11.8 F. Albarracín: Machine learning techniques to construct and explore skyrmion phase diagram

11:20 1.18 N. Ezzell: A black-box quantum Monte Carlo approach to quantum phase transitions and more

Breakout 2

8:00 1.19 D. Dao: Molecular Dynamics Study of Interface Bonding Transition in Transition Metal Dichalcogenide Lateral Heterostructures

8:20 1.27 N. Akutsu: Asymmetric fluctuations of growth/retreat on the Kardar-Parisi-Zhang-like surface kinetic roughening for steady crystal growth/retreat

8:40 1.33 A. Lotfalinezhad: Effects of nanochannel geometry and surface properties on water permeation: A molecular dynamics study

9:00 1.36 H. Darestani: Molecular Dynamics Study on the Role of Graphene Coating in Mitigating Cavitation-Induced Damage on a Metallic Surface

9:20 1.35 P. Bhandari: Non-equilibrium steady-state dynamics in the Coulomb glass model

9:40 2.6 V. Malik: Coarsening dynamics and aging of a two-dimensional Coulomb Glass Model

10:00 2.8 M. Weigel: Low-energy excitations in spin glasses

10:20 1.26 D. Pereira: Kinetic magnetism in the crossover between the square and triangular lattice Fermi-Hubbard models

10:40 2.1 N. Fytas: Universal exotic dynamics in critical mesoscopic systems

11:00 1.32 D. Warkotsch: Harnessing finite-size effects to gauge aging in the 2D Ising model

11:20 11.9 M. Zhang: A Generalized Framework for Alchemical Machine-Learned Interaction Models in Coarse-Grained Polymer-Grafted Nanoparticle Self-Assembly

Committees

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Plenary Lectures

Tuesday, 10:00am, plenary

Jack Dongarra

Professor Emeritus

Electrical Engineering and Computer Science Department, Innovative Computing Laboratory

University of Tennessee, Knoxville

dongarra@icl.utk.edu

Superintelligence for scientific discovery

Wednesday, 12:00 noon, plenary

Markus J. Buehler
McAfee Professor of Engineering
Massachusetts Institute of Technology
mbuehler@mit.edu

AI is rapidly transitioning from a passive analytical assistant to an active, self-improving partner in scientific discovery. In the material world, this shift means developing systems that not only recognize patterns but also reason, hypothesize, and autonomously explore new ideas for design, discovery and manufacturing. This talk presents emerging approaches toward 'superintelligent' discovery engines -integrating reinforcement learning, graph-based reasoning, and physics-informed neural architectures with generative models capable of cross-domain synthesis and in-situ learning. We explore multi-agent swarm systems inspired by collective intelligence in nature, enabling continuous self-evolution as they solve problems. Case studies from materials science, engineering and biology illustrate how these systems can uncover hidden structure-property relationships, design novel materials, and accelerate innovations in sustainability engineering and beyond. These advances chart a path toward AI that actively expands the boundaries of human knowledge.

Engineering Quantum Materials via Cavity Vacuum Fluctuations: an ab initio QEDFT framework

Wednesday, 10:00am, plenary

Angel Rubio

Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany

Initiative for Computational catalysis (ICC) and Center for Computational Quantum Physics (CCQ) Flatiron Institute, 10010 NY, USA

A central challenge in computational physics is developing accurate, efficient theories for light-driven, non-equilibrium phenomena and emergent quantum states. Time-Dependent Density Functional Theory (TDDFT) has been crucial for modeling light-induced changes in complex systems, but extending this to strongly coupled light–matter regimes requires new tools. Quantum Electrodynamics Density Functional Theory (QEDFT) provides a first-principles framework to predict and control ordered phases in hybrid electron–photon systems. This foundation defines Cavity Materials Engineering—the design of novel quantum states through strong electron–photon coupling and quantum vacuum fluctuations. In this “dark” regime, matter ground states can be reshaped without real photon excitation, enabling vacuum-driven quantum phase transitions. Rooted in non-relativistic QED, QEDFT unifies light–matter interactions with electronic structure, opening paths to engineer phases such as cavity-enhanced superconductivity, fractional quantum Hall states, and topological materials. We close by highlighting key theoretical and computational challenges for this emerging field.

Simulating magnetized supermassive black hole feedback at the exascale

Wednesday, 11am, plenary

Brian W. O'Shea

Department of Computational Mathematics, Science, and Engineering

Department of Physics and Astronomy

Michigan State University

oshea@msu.edu

Galaxy clusters are the most massive virialized objects in the universe, with masses hundreds to thousands of times that of our own Milky Way and physical scales extending for millions of light years. The bulk of the baryons contained within these systems is comprised of a hot, diffuse, and magnetized plasma that glows brightly in X-ray wavelengths. The energy radiated away by X-rays is replaced by heating from active galactic nuclei, which are relativistic jets powered by accretion onto the supermassive black hole in the cluster's central galaxy (also referred to as an "Active Galactic Nucleus", or AGN), maintaining the system in a dynamic equilibrium. This heating occurs through interactions of the AGN jet with the intracluster medium, which ultimately is transported throughout the highly X-ray luminous cluster core. In this talk I will explain how we simulate systems of this type, which span a huge dynamical range in space and time. I will also present results from the XMAGNET exascale magnetohydrodynamics simulations of idealized galaxy clusters with a cold gas accretion-fed, magnetized AGN jet in the center. I will explain the mechanisms by which cold gas triggers the AGN jet and how the heating from this jet regulates the amount of cold gas in the system. I will also discuss in detail the generation of turbulence by the magnetized jet, the amplification of the ambient cluster magnetic fields by turbulence-driven dynamos, and the formation of multiphase gas (which is created via thermal instability) and its relationship with the cluster magnetic fields.

IUPAP C20 Early Career Prize in Computational Physics

Thursday, 12noon, plenary

Felipe H. da Jornada

Department of Materials Science and Engineering

Stanford University

jornada@stanford.edu

Contributed Talks

1.1: Superconducting properties of Fe/Au/Nb heterostructures form first principles

Monday, 8:10am, Breakout 1

B. Ujfalussy, G. Csire

Submitted by:*Balazs Ujfalussy; ujfalussy.balazs@wigner.hu; HUN-REN Wigner Research Centre for Physics*

We generalize the fully relativistic screened Korringa-Kohn-Rostoker (SKKR) method for solving the corresponding Kohn-Sham-Dirac-Bogoliubov-de Gennes (KSDBdG) equations for surfaces and interfaces. As an application, we study the quasiparticle spectrum of Au overlayers on Nb host. We find that, within the superconducting gap region, the quasiparticle spectrum consists of Andreev bound states (ABS) with a dispersion that is closely connected to the underlying electronic structure of the overlayer. When combined with a semi-phenomenological parameterization of the electron-phonon coupling, a material-specific model arises to calculate the superconducting critical temperature from the thickness dependence. In the case of Au/Nb heterostructures, we obtain a very good agreement with experiments. Moreover, predictions are made for similar heterostructures of other compounds. Extending our calculations to Fe-covered Nb and Nb/Au multilayers, we show that the order parameters exhibit a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) like oscillations in the iron layers, but more interestingly, an oscillatory behaviour is observed in the gold layers as well. The band structure calculations suggest that this is the consequence of an interplay between the quantum-well states and ferromagnetism, and show a rather similar oscillatory behavior of the critical temperature observed in experiments. Similarly, experiments in epitaxial Nb/Au/Nb trilayers show that the critical current density, the superconducting coherence length, and the superconducting transition temperature all show an oscillating behavior as a function of the Au-layer thickness. Such behavior cannot be understood based on simple models of the Josephson effect. Using first principles theory, we study the effects of spin-orbit coupling and the effect of confinement, and show that they induce a complex structure of Andreev states in the superconducting state ,which in turn modifies the quasiparticle spectrum and the Josephson supercurrent. Our study reveals the coexistence of two superconducting phases in the gold layers, the usual intraband s-wave phase and an additional FFLO phase stemming from interband pairing (without a magnetic field). The results indicate the rich interplay between quantum size and proximity effects, which suggests the possibility of modifying superconducting transport properties by exploiting thickness-dependent quantum size effects.

1.2: Electrically-tunable ultra-flat bands and π-electron magnetism in graphene nanoribbons

Tuesday, 8:20am, Breakeout 1

Michele Pizzochero, Ruize Ma, Nikita Tepliakov, Arash Mostofi

Submitted by:*Michele Pizzochero; mp2834@bath.acuk; Department of Physics, University of Bath, UK*

Atomically thin crystals with flat electronic bands have recently emerged as key platforms for exploring and engineering strongly correlated states. However, the range of low-dimensional flat-band materials remains relatively limited, primarily confined to two-dimensional moiré superlattices. In this work, we predict the formation of reversible, electrically induced ultra-flat bands and -electron magnetism in one-dimensional chevron graphene nanoribbons using ab initio calculations. We show that applying a transverse electric field to these nanoribbons generates a pair of isolated, nearly perfectly flat bands with bandwidths of approximately 1 meV, symmetrically centered around the Fermi level. Upon charge doping, these flat bands exhibit a Stoner-like electronic instability, leading to the emergence of local magnetic moments at the edges of the otherwise non-magnetic nanoribbon, ultimately forming a one-dimensional spin-1/2 chain. Our findings broaden the range of carbon-based nanostructures exhibiting flat bands and provide new strategies for inducing correlated electronic phases in chevron graphene nanoribbons.

1.3: First-principle simulations of hybrid interfaces: N-heterocyclic carbenes and olefins on metal surfaces and 2D materials

Tuesday, 8:40am, Breakout 1

Masoumeh Alihosseini (University of Milan), Shamik Chakraborty (University of Milan), Shuangying Ma (University of Milan), Elena Molteni (University of Milan), Guido Fratesi(*) (University of Milan)

Submitted by: *Guido Fratesi; guido.fratesi@unimi.it; University of Milan, Italy*

N-heterocyclic carbenes (NHCs) are a fascinating class of compounds characterized by a divalent carbon atom within a nitrogen-containing heterocyclic ring. This unique structure provides NHCs with remarkable stability and reactivity, distinguishing them from traditional carbenes, which are often transient and highly reactive. NHCs have use in various felds of chemistry and materials science, as they serve for example as very good ligands to different species. NHCs are found useful to modify surfaces, especially gold and other metals, creating robust hybrid interfaces. In this talk I will review our recent and ongoing theoretical studies, based on ab initio Density Functional Theory (DFT), of the hybrid interfaces formed by NHCs and related molecules with metals, 2D materials such as transition-metal trihalides and graphene, and organometallic species (porphyrins). In collaboration with experimental groups, we have studied the adsorption of N-heterocyclic olefins (NHOs, derivatives of NHCs featuring an exceptionally electron rich and strongly polarizable double bond) on Au(111) [1]. DFT structural optimizations yield for both molecules at-lying adsorption geometries as the preferred ones, in agreement with measured near-edge X-ray absorption ne structure spectra (NEXAFS). We demonstrate that adsorption occurs at a gold adatom via the CH2 carbon, so that NHOs take the ylidic form on the surface, and that the NHO-Au-adatom complex is the base entity of the observed self-assembled overlayers. We have then focused on meso-ionic carbenes (MICs) still on Au(111), demonstrating by measured and simulated NEXAFS, total energy calculations and molecular dynamics simulations, that also in this case the MIC-Au-adatom binding is essential to stabilize the interface. I will report on our study of NHCs on CrI3. In this case, we nd that NHC adsorbs vertically with the electron rich carbene C above an I atom, lifting it from the substrate and leading to several electronic modifications at the interface: charge loss on I, increased magnetic moments on surrounding Cr atoms, a net substrate moment increase of 2 μB/NHC, and the emergence of two localized states within the band substrate gap. [1] Berg et al., Angew. Chem. Int. Ed. 62 (2023) e202311832 [2] Berg et al., Nanoscale (2025) in press 10.1039/d5nr02802g Work funded by the European Union's Horizon 2020 Research and Innovation program under grant agreement no. 101077332 "NFFA-Europe-Pilot", and Next Generation EU - "PNRR - M4C2, investimento 1.1 - "Fondo PRIN 2022" - FUnctionalized surfaces by True molecUlar bottom-up gROwth (FUTURO) id 2022FWZCHK – CUP G53D23002960006.

1.4: Collective nature of phonon energies beyond harmonic oscillators

Thursday, 10:00am, Breakout 1

Jaeyun Moon

Submitted by:*Jaeyun Moon; jaeyun.moon@ufl.edu; University of Florida*

Phonon quasi-particles have been monumental in microscopically understanding thermodynamics and transport properties in condensed matter for decades. Phonons have one-to-one correspondence with harmonic eigenstates and their energies are often described by simple independent harmonic oscillator models. Higher order terms in the potential energy lead to interactions among them, resulting in finite lifetimes and frequency shifts, even in perfect crystals. However, increasing evidence including constant volume heat capacity violating the Dulong-Petit law suggests the need for re-evaluation of phonons as having independent harmonic energies. In this work, we explicitly examine inter-mode dependence of phonon energies of a prototypical crystal, silicon, through energy covariance calculations and demonstrate the concerted nature of phonon energies even at 300K, questioning independent harmonic oscillator assumptions commonly used for phonon energy descriptions of thermodynamics and transport.

1.5: Data-driven high-throughput search for the accelerated discovery of rare-earth-free permanent magnets

Wednesday, 8:00am, Breakout 1

Junaid Jami, Nitish Bhagat, Amrita Bhattacharya

Submitted by:*Md Junaid Afsar Jami; junaid.jami777@gmail.com; Indian Institute of Technology Bombay*

An integrated data-driven approach combined with a high-throughput framework based on first principles calculations was employed to discover novel rare-earth-free permanent magnets, focusing on binary alloys. Compounds were systematically screened based on their elemental composition, structure, stability, and magnetization. Density functional theory (DFT) calculations were performed on selected candidates to evaluate their magnetocrystalline anisotropy energy (MAE) and Curie temperature (TC), leading to the identification of ten promising materials. Out of these, a thorough literature review confirmed the novelty of ZnFe, while Fe8N corresponds to the well-known Fe16N2 phase, extensively investigated in thin-film form, but with limited data available for its bulk counterpart. Our computational analysis addresses this gap by providing valuable insight into its bulk magnetic properties, thereby supporting its continued relevance as a high-performance rare-earth-free magnet and reinforcing the effectiveness of our screening strategy. Their ferromagnetic ground state was verified via DFT, and structural stability confirmed through negative formation enthalpies, phonon spectra, and elastic criteria. Tetragonal ZnFe and Fe8N exhibit high saturation magnetization (>1 T), large anisotropy constants (>0.5 MJ/m3), and high TC (>1200 K). Their magnetic hardness parameters (= 0.85 for ZnFe and 0.70 for Fe8N) further support their potential as gap magnets. These findings underscore the effectiveness of our high-throughput screening strategy, offering a theoretical blueprint for the experimental realization of rare-earth-free permanent magnets.

1.6: Engineering Electronic Properties of 2D Materials for Enhanced Supercapacitor Performance

Tuesday, 9:00am, Breakout 1

Sruthi T and Vincent Mathew

Submitted by:*Dr. Sruthi T.; drsruthi2023@gmail.com; Central University of Kerala, India*

Sruthi T and Vincent Mathew Computational Nanoscience Lab, Department of Physics, Central University of Kerala, India Corresponding author: drsruthi2023@gmail.com Abstract Efficient and sustainable energy storage remains a central challenge in advancing renewable energy technologies. Two-dimensional (2D) supercapacitors, with their high ion density, long cycle life, and rapid charge–discharge capability, are emerging as promising candidates for next-generation storage systems. In this work, we investigate the quantum capacitance (CQ) of MoSe monolayers functionalized with transition metal (TM) ad-atoms using density functional theory (DFT) within the Vienna Ab initio Simulation Package (VASP). Our calculations reveal that pristine MoSe, being a direct-band semiconductor with no states near the Fermi level, exhibits negligible CQ. However, substitutional doping with TM ad-atoms such as Mo, Nb, Ta, and Tc induces significant charge redistribution, leading to the emergence of electronic states near the Fermi level. This modification alters the carrier concentration, shifts the Fermi level, and results in a substantial enhancement of CQ, with values exceeding 500 µF/cm^2—significantly higher than previously reported results. These findings demonstrate that ad-atom functionalization of MoSe monolayers can effectively tune electronic structures, thereby nanoengineering their quantum capacitance for superior supercapacitor performance. Keywords: Supercapacitors, Energy storage, Quantum capacitance, 2D materials, Electronic structure, Density functional theory

1.7: Impact of Water Content on the Mechanical and Thermodynamic Properties of Phosphonium Ionic Liquids

Monday, 8:10am, Breakout 2

Miljan Dašić, Igor Stanković, Mateja Jovanović, Ashlie Martini

Affiliation of Miljan Dašić, Igor Stanković, and Mateja Jovanović: Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, Belgrade (Serbia)

Affiliation of Ashlie Martini: Department of Mechanical Engineering, University of California Merced, Merced, California (United States of America)

Submitted by:*Miljan Dašić; mdasic@ipb.ac.rs; Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, Belgrade (Serbia)*

Phosphonium-based Room-Temperature lonic Liquids (RTILs) have been gaining an increasing attention due to their unique physicochemical properties, which make them suitable for applications regarding lubrication, electrochemistry, and green chemistry. However, their behavior is significantly influenced by the water content, which alters their mechanical and thermodynamic properties. Taking this fact into account, we conducted extensive All-Atom Molecular Dynamics simulations, in order to investigate how varying water content affects the transport and thermodynamic properties of the three representative phosphonium-based RTILs. By analyzing the structural, transport, as well as energetic characteristics of these ionic liquids, we provide detailed insights into the fundamental mechanisms governing their dynamic behavior in the presence of water.

Our study focuses on the key transport properties, such as viscosity and self-diffusion coefficients, and their dependence on water concentration. We have observed that increase of water content significantly enhances ion mobility by disrupting ion-ion interactions. Water molecules preferentially interact with ionic species, hence effectively reducing Coulombic interactions and hydrogen bonding networks within the ionic liquid. This weakening of electrostatic forces leads to: a noticeable decrease in viscosity, and also to a noticeable increase in diffusion coefficients, thus highlighting the critical role of water content in these systems.

Additionally, we examined the thermodynamic stability of the studied ionic liquids mixed with water by analyzing interaction energies and phase behavior. Presence of water leads to a decrease of cohesive energy density, hence resulting in a lower boiling point and increased volatility, compared to the boiling point and volatility of a pure ionic liquid. These findings suggest that phosphonium-based ionic liquids exhibit a water-dependent transition of their structure, which influences their macroscopic properties.

Results regarding phosphonium ionic liquids were compared with the well-studied 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim]+ [PF6]-) ionic liquid, which was used as a reference. Our comparative analysis revealed that phosphonium ionic liquids exhibit distinct water interaction patterns due to their larger, more hydrophobic cation structure. This distinction provides critical insights into their suitability for specific applications where water tolerance or exclusion is required.

Our study underscores the importance, and even necessity, of considering the water content when designing and selecting phosphonium ionic liquids for practical applications. Besides that, our findings significantly contribute to the broader understanding of how do molecular-scale interactions govern the macroscopic properties of ionic liquids, tracing the way for improved formulations tailored for industrial applications of ionic liquids in the fields like: tribology, solvent design, electrochemistry, etc. By elucidating the intricate role which water plays in mixtures with phosphonium ionic liquids, our work provides a foundation for optimizing the performance of such RTILs in various scientific and engineering/technological fields.

1.8: Switchable Chern number in van der Waals heterostructures

Wednesday, 9:20am, Breakeout 1

Amarjyoti Choudhury Cesare Cozza Marco Gibertini

Submitted by:*AMARJYOTI CHOUDHURY; achoudhury@unimore.it; Department of Physics, University of Modena and Reggio Emilia, Via G. Campi 213/A, 41125 Modena, Italy*

Despite the huge expansion in the family of 2D materials, Chern insulators remain rare, with most monolayers being topologically trivial. However, stacking such trivial materials into van der Waals heterostructures offers vast opportunities for emergent topological phases. Here we show how to engineer topological heterostructures from trivial layers and control their Chern number via an external magnetic field. The key is combining ferromagnetic monolayers–whose valence band edge depends on magnetization direction–with trivial semiconductors having suitable band alignment. This can induce a band inversion–and a topological transition–for one magnetization orientation but not the other, enabling field-tunable topological order. The theoretical scenario is validated through accurate first-principles simulations by screening 2D databases for realistic materials platforms. We acknowledge financial support from the EMPEROR project, CUP E93C24001040001, funded by the European Union—NextGeneration EU (M4C2INV1.3) through the National Quantum Science and Technology Institute (Spoke 5).

1.9: Ultralow Lattice Thermal Conductivity and Colossal Thermoelectric Figure of Merit of the Room Temperature Antiferromagnet CsMnBi

Tuesday, 12:00, Breakout 1

Shubham Rakesh Singh, Nirpendra Singh, Udo Schwingenschlögl

Submitted by:*Shubham Rakesh Singh; shubham.singh@kaust@kaust.edu.sa; KAUST*

We study the experimentally synthesized layered material CsMnBi using first-principles calculations and the linearized electron and phonon Boltzmann transport equations. CsMnBi is found to be a semiconductor with a indirect bandgap of 0.9 eV and to realize C-type antiferromagnetism, which is energetically favorable by 187 meV per formula unit over ferromagnetism. Energetical overlap between the acoustic and low-frequency optical phonon modes enhances the phonon-phonon scattering. Combined with low group velocities and high lattice anharmonicity this results in an ultralow lattice thermal conductivity of 0.07 Wm^1K^1 at 300 K. A high thermoelectric figure of merit of 2.2 (1.7) is achieved at 300 K at a hole (electron) density of $6.0 \times 10^{18} (1.0 \times 10^{18}) cm^3$.

1.10: Crystallographic orderings in refractory high-entropy superalloys studied via an ab initio concentration wave analysis and atomistic Monte Carlo simulations

Wednesday, 8:20am, Breakeout 1

Christopher D. Woodgate, Hubert J. Naguszewski, David Redka, Jan Minar, David Quigley, Julie B. Staunton

Submitted by: *Christopher Woodgate; christopher.woodgate@bristol.ac.uk; University of Bristol*

Refractory high-entropy superalloys (RSAs) are metallic alloys containing aluminium and at least three further early transition metal elements. Although in general high-entropy alloys are expected to form single-phase solid solutions in which all lattice sites have uniform probabilities of being occupied by different elements, the addition of Al as an alloying element is understood to promote the formation of crystallographically ordered structures. Here, we combine ab initio electronic structure calculations, a concentration wave analysis, and atomistic simulations to examine the phase stability of two prototypical RSAs: AlTiVNb and AlTiCrMo [1]. In alignment with experimental observations, we predict B2 crystallographic orderings emerging at high temperatures in both alloys, as well as eventual decomposition into multiple competing phases with decreasing temperature. We interpret these findings in terms of the alloys' underlying electronic structure, with hybridisation between the sp states of Al and the d states of the transition metals understood to play an important role. We then examine the impact of these crystallographic orderings on the alloys' residual resistivity. Counterintuitively, for both alloys, we find that the emergence of (partial) long-range crystallographic order results in an increase in residual resistivity. We understand this increase as originating in a reduction in the electronic density of states at the Fermi level induced by the ordering, as well as qualitative changes to the nature of the alloys' smeared-out Fermi surfaces.

[1] C. D. Woodgate et al., Journal of Physics: Materials 8, 045002 (2025).

1.11: Investigation of Piezoelectric Properties of Galfenol - PVDF Interface Using Density Functional Theory

Friday, 8:00am, Breakeout 1

T Kulawardena

L S I Liyanage

A A G A Abeygunawardena

Submitted by: *Tharin Kulawardena; tkulawardana1@gmail.com; College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya, Sri Lanka*

The design of hybrid piezoelectric–magnetostrictive interfaces presents a promising pathway for next-generation biomedical devices, particularly in bone healing applications where mechanical stimulation can accelerate bone regeneration. This study investigates the piezoelectric response of a Galfenol–PVDF (FeGa–polyvinylidene fluoride) interface using first-principles Density Functional Theory (DFT) calculations performed with Quantum Espresso. The primary objective was to understand how interfacial strain, layer thickness, and electronic interactions influence the polarization behavior and overall piezoelectric performance of the interface system. Fully optimized bulk Galfenol and PVDF structures were used to construct the interface. The interface was structurally optimized and its electronic structure was analyzed through band structure and density of states (DOS) calculations. Berry phase calculations were employed to evaluate spontaneous polarization of both bulk and interface structures. Three lattice strains between Galfenol and PVDF were introduced and the electronic structure and polarization change was investigated. Also, the influence of layer thickness on the electronic properties were investigated. The results revealed that both strain and thickness have a pronounced effect on polarization. Bulk PVDF exhibited a polarization of 0.1791 C/m^2, while the Galfenol–PVDF interfaces displayed values ranging from 0.0348 C/m^2 under tensile strain to +0.0529 C/m^2 under compressive strain. Under tensile train and compressive strain conditions piezoelectric stress tensor ranged from -0.3703C/m2 to +0.8614 C/m^2. Increasing the thickness of the Galfenol and PVDF layers further enhanced dipole alignment and polarization, confirming that layer geometry plays a critical role in improving the interfacial piezoelectric response. Electronic structure analysis indicated partial charge leakage across the interface due to metallic states in Galfenol, which slightly reduced the effective polarization. Overall, this study demonstrates that optimizing interfacial strain

and layer geometry can significantly enhance the piezoelectric response of the Galfenol–PVDF interface, supporting its potential application in piezoelectric-based bone healing devices that convert mechanical stress into bioelectric signals to promote bone regeneration.

1.12: Investigation of the Proton Transport Mechanism in Sc-Doped CaZrO3 Using Ab-Initio Molecular Dynamics Simulations

Tuesday, 12:40pm, Breakout 2

Sanjib Ray ; P. Padma Kumar

Submitted by:*Sanjib Ray; sray@iitg.ac.in; Indian Institute of Technology Guwahati*

Perovskite-based protonic conductors are promising electrolyte materials for solid oxide fuel cells. Although numerous studies have been conducted in these systems, many microscopic aspects related to proton transport are still unknown. We present ab initio molecular dynamics studies of proton transport in Sc-doped CaZrO3 to gain insights into proton conduction mechanisms. It is noted that the proton transfer along the two primary channels, namely, intraoctahedral and interoctahedral, is sensitive to the local cationic environments. While the proton hops in the Zr–O(H)–Zr environments are predominantly interoctahedral hops, the Zr–O(H)–Sc environments promote both channels alike. However, the interoctahedral proton hops from the Zr–O(H)–Sc environments are followed by persistent jump-reversals leading to the localization of the protons, with negligible contribution to the ionic conductivity. Exploiting the van-Hove correlation functions, it is demonstrated that the nature of the localization essentially involves proton scrambling over the ScO6 octahedra, unlike earlier perceptions.

The Journal of Physical Chemistry C (DOI:https://doi.org/10.1021/acs.jpcc.4c08036).

1.13: Simulation of scanning tunneling microscopy and spectroscopy from first principles beyond the Tersoff-Hamann approximation

Monday, 8:30am, Breakout 1

Krisztian Palotas

Submitted by:*Krisztian Palotas; palotas.krisztian@wigner.hu; HUN-REN Wigner Research Center for Physics, Budapest, Hungary*

Understanding and engineering scanning tunneling microscopy (STM) image contrasts and scanning tunneling spectroscopy (STS) sensitivity are of crucial importance in wide areas of surface science and related technologies, ranging from magnetic surfaces to molecular structures. In many cases going beyond the Tersoff-Hamann approximation is essential. In the talk a few electron tunneling theories are introduced for the purpose of high-resolution simulation of STM and STS. These theoretical methods rely on electronic structure data obtained from first principles, and are implemented in two STM program packages: BSKAN [1,2] and 3D-WKB-STM [3]. A practical introduction to the usage of these STM simulation codes based on DFT-based electronic structure data is briefly given, followed by selected examples on different STM tip effects on the STM imaging mechanism: (i) the role of tip-orbital interference within the revised Chen's derivative rules [4,5], and (ii) asymmetric/tilted tip orientation effects [5,6]. Going beyond scalar charge current in spin-polarized STM, a combined tunneling electron charge and vector spin - longitudinal spin current and spin transfer torque - transport theory is presented, with application to magnetic skyrmions [7].

[1] W. A. Hofer, Prog. Surf. Sci. 71, 147 (2003) [2] K. Palotás, W. A. Hofer, J. Phys. Condens. Matter 17, 2705 (2005) [3] K. Palotás et al., Front. Phys. 9, 711 (2014) [4] G. Mándi, K. Palotás, Phys. Rev. B 91, 165406 (2015); I. Abilio, K. Palotás, Phys. Rev. B 111, 245425 (2025) [5] I. Abilio et al., Phys. Rev. B 110, 125422 (2024) [6] G. Mándi et al., J. Phys. Condens. Matter 24, 445009 (2013), J. Phys. Condens. Matter 26, 485007 (2014), Prog. Surf. Sci. 90, 223 (2015) [7] K. Palotás et al., Phys. Rev. B 94, 064434 (2016), Phys. Rev. B 96, 024410 (2017), Phys. Rev. B 97, 174402 (2018), Phys. Rev. B 98, 094409 (2018), J. Magn. Magn. Mater. 519, 167440 (2021)

1.14: Scalable First Principles Calculations for Alloys

Monday, 9:10am, Breakout 1

Markus Eisenbach

Submitted by:*Markus Eisenbach; eisenbachm@ornl.gov; National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831*

The effect of disorder in materials is of great fundamental and technological interest. Here I will present our implementation of multiple scattering theory for first principles density functional calculations. This approach directly obtains the single particle Green's function of the Kohn-Sham equation, either in reciprocal space (Korringa-Kohn-Rostocker i.e. KKR) or real space (Localy-Selfconsistent Multiple Scattering i.e. LSMS). The KKR method allows an efficient description of random solid solution alloys using the Coherent Potential Approximation (CPA), while our LSMS code allows for scalable large scale first principles density functional calculations of materials. A fundamental science driver for scalable, large scale, first principles calculations of materials is the need to understand states beyond periodic crystalline lattices. For large simulation cells, needed to describe extended electronic and magnetic orderings, defect states or disorder in alloys, the cubic scaling of traditional first principles methods have prevented direct calculations. The linear scaling nature of the LSMS ab initio code enables the treatment of extremely large disordered systems from the first principles using the largest parallel supercomputers available, such as calculations for O(10,000 - 100,000) atoms on current high performance computing architectures. For exascale systems, we have extended the use of accelerators to enable the efficient calculation for embedding methods and forces. Currently ongoing work focuses on the calculation of electric conductivity in the presence of disorder and defects.

While DFT calculations have proven to be a useful tool in the study of ground state properties of many materials, we will go beyond the ground state by describing an approach to utilize machine learning methods to combine first principles density functional calculations with classical Monte-Carlo simulations to investigating the statistical mechanics of materials. The investigation of finite temperature properties relies on the possibility of a large number of evaluations of the system's Hamiltonian that are required to sample the phase space needed to obtain physical observables. We have demonstrated a solution to this problem that harnesses the computational power of large massively parallel computers by combining classical Monte-Carlo calculations with our first principles multiple scattering electronic structure code (LSMS) by employing Machine Learning techniques.

The combination of LSMS with a machine learning workflow, that can consider both classical interaction models and artificial neural network based models, allows us to investigate alloy ordering transitions for increased simulation cell sizes. Our approach can sample both magnetic or chemical order, allowing the first principles calculation of order/disorder phase transitions and phase separations in alloys.

These computational capabilities are available in our Multiple Scattering Theory suite (MuST) [https://github.com/mstsuite]

This work was supported in part by the Office of Science of the Department of Energy and by the Laboratory Directed Research and Development (LDRD) Program of Oak Ridge National Laboratory. This research used resources of the Oak Ridge Leadership Computing Facility, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

1.15: Semi-Empirical Pseudopotential Method for Low-Dimensional Materials

Tuesday, 8:00am, Breakout 1

Dr. Raj Kumar Paudel Prof. Chung-Yuan Ren Prof. Yia-Chung Chang

Submitted by:*Raj Kumar Paudel; rajupdl6@phys.ncku.edu.tw; Department of Physics, NCKU, Tainan*

Semi-Empirical Pseudopotential Method for Low-Dimensional Materials Raj Kumar Paudel1,3, Chung-Yuan Ren2, and Yia-Chung Chang1,3 1Research Center for Applied Sciences, Academia Sinica, Taipei 115 2Department of Physics, National Kaohsiung Normal University, Kaohsiung 824, Taiwan 3Department of Physics, National Cheng Kung University, Tainan 701, Taiwan

Modeling realistic 2D material devices is crucial for next-generation nanoelectronics, but DFT calculations become prohibitively expensive for systems with thousands of atoms—a scale required for moiré superlattices and nanoribbon devices. We have developed an efficient semi-empirical pseudopotential (SEPM) method [1,2] that performs one high-quality DFT calculation, fits the effective potential to analytical functions, and then directly solves the Schrödinger equation without self-consistency iterations. Using a mixed basis of 2D plane waves and B-spline functions, our method reproduces DFT [3] band structures with high accuracy while running orders of magnitude faster. We demonstrate the method's versatility across three material systems. For graphene, we reproduce the Dirac cone and -bonded states. For armchair graphene nanoribbons, a simple edge-correction potential accounts for charge redistribution, accurately predicting bandgaps that match experimental values (7-AGNR: 1.43 eV; 9-AGNR: 0.68 eV). We have now extended this framework to monolayer TMDCs (MoS, MoSe, WS, WSe), where despite their complex multi-atom unit cells and d-orbitals, we achieve excellent agreement with DFT (MoS bandgap: 1.82 eV vs. DFT 1.80 eV). This unified framework makes previously impractical calculations of large moiré superlattices and device optimizations feasible, with extensions for spin-orbit coupling and transport properties underway.

References [1] Paudel, R.K.; Ren, C.-Y.; Chang, Y.-C. Semi-Empirical Pseudopotential Method for Graphene and Graphene Nanoribbons. Nanomaterials 2023, 13,2066 [2] Paudel, R. K.; Ren, C.-Y.; Chang, Y.-C. Semi-empirical Pseudopotential Method for Monolayer Transitional-Metal Dichalcogenides. arXiv preprint arXiv:2506.11360, 2025. [3] Chung-Yuan Ren, Chen-Shiung Hsue and Yia-Chung Chang. A mixed basis density functional approach for low dimensional systems with B-splines. Computer Physics Communications 188 (2015), pp. 94–102.

1.16: Efficient real-space Hubbard-corrected density functional theory (DFT+U) with U from Hybrid functionals

Monday, 8:50am, Breakeout 1

Sayan Bhowmik; Andrew J. Medford; Phanish Suryanarayana

Submitted by:*Sayan Bhowmik; sbhowmik9@gatech.edu; Georgia Institute of Technology*

A highly efficient and accurate real-space framework for Hubbard-corrected Density Functional Theory (DFT+U) is presented. This framework features a finite-difference formulation of the energy, forces, and stress tensor, implemented in the scalable, highly parallel DFT code SPARC. Performance benchmarks demonstrate that our real-space approach achieves greater than an order-of-magnitude speedup compared to standard planewave methods, a critical advantage for large-scale systems. Further, we examine the exchange-correlation consistency of local orbital generation and introduce a novel scheme for self-consistently optimizing the Hubbard U parameter using hybrid functionals, with demonstrated application to various TiO_2 polymorphs.

1.17: Transition Metal Doping and Strain as Dual Pathways to Control Adhesion and Conductivity in RuO_2

Friday, 8:20am, Breakout 1

Mehmet Gokhan Sensoy

Submitted by:*Mehmet Gokhan Sensoy; mehmet.sensoy@erdogan.edu.tr; Recep Tayyip Erdogan University*

Ruthenium dioxide (RuO_2) has emerged as one of the most promising conductive oxides for micro- and nano-electromechanical systems (MEMS/NEMS) due to its high electrical conductivity, chemical stability, and resistance to oxidation. However, tailoring its interfacial and electronic properties remains essential for improving device reliability, reducing wear, and enhancing energy efficiency. In this work, we employ density functional theory (DFT) calculations to systematically investigate how transition metal (TM) doping and strain engineering can be used to tune the electrical and adhesion properties of RuO_2. Formation energy calculations reveal that dopants such as Mn and Fe are energetically favorable within the RuO_2 lattice, while noble metals such as Au and Cd introduce instability and deteriorate electronic performance. The Kubo–Greenwood formalism was used to determine the electrical conductivity of doped structures, showing that Mn doping up to 6% maintains high conductivity, whereas excessive concentrations or heavy dopants significantly reduce it. Electronic density of states analyses indicate that Mn and Fe introduce additional d-states near the Fermi level, increasing carrier density and thereby enhancing conductivity. Adhesion behavior was studied for RuO_2 (110) surfaces under both doped and strained conditions. Moderate Mn doping (2%) increased adhesion energy to 0.13 J/m² compared to 0.08 J/m² for pristine RuO_2, while higher doping levels led to reduced adhesion due to increased electronic repulsion. The application of compressive strain further strengthened adhesion, whereas tensile strain weakened interfacial bonding, highlighting the tunability of mechanical interactions through strain modulation. Our findings demonstrate that combining transition metal doping with strain engineering provides an effective strategy to optimize both electrical and interfacial properties of RuO_2. These results offer valuable insights for designing stable and low-adhesion RuO_2-based contact materials for MEMS/NEMS switches, where controlled adhesion and high conductivity are critical for performance, durability, and device miniaturization.

1.18: A black-box quantum Monte Carlo approach to quantum phase transitions and more

Friday, 11:20am, Breakeout 1

Nic Ezzell, Lev Barash, and Itay Hen

Submitted by:*Nic Ezzell; naezzell@gmail.com; USC*

We derive exact, universal, closed-form quantum Monte Carlo estimators for finite-temperature energy susceptibility and fidelity susceptibility, applicable to essentially arbitrary Hamiltonians. Combined with recent advancements in Monte Carlo, our approach enables a black-box framework for studying quantum phase transitions–without requiring prior knowledge of an order parameter or the manual design of model-specific ergodic quantum Monte Carlo update rules. We demonstrate the utility of our method by applying a single implementation to the transverse-field Ising model, the XXZ model, and an ensemble of models related by random unitaries. Time permitting, we show how these results can be generalized to estimate essentially arbitrary observables.

1.19: Molecular Dynamics Study of Interface Bonding Transition in Transition Metal Dichalcogenide Lateral Heterostructures

Friday, 8:00am, Breakout 2

Duy Minh Dao, Mahdi Ghorbani-Asl

Submitted by:*Duy Minh Dao; daoduy.work@gmail.com; Vietnam National University - Ho Chi Minh University of Technology*

Lateral heterostructures are highly promising materials because introducing interfacial defects can significantly alter the properties of the pristine material. This study employs the Stillinger-Weber empirical potential within molecular dynamics simulations to investigate the structural transition of lateral heterostructures formed by pairs of sulfide-based transition metal dichalcogenides (TMDs). Specifically, we determine the transitional, or critical width, at which the coherent interface switches to a dislocated-type interface. Furthermore, we examine the ripple formation characteristic of the dislocated structures, focusing on their energy gain and the change in their elevation with respect to temperature. Our results draw a direct correlation between the nature of this ripple formation and the underlying interface bonding mechanism.

1.20: Atomistically-Informed Modelling of Dislocation Loops in Tungsten

withdrawn

Joseph Duque, Sergei Dudarev, James Kermode, Thomas Hudson

Submitted by:*Joseph Duque; Joseph.Duque@warwick.ac.uk; University of Warwick*

Atomistic simulations using Density Functional Theory can only capture femtoseconds worth of data within a limited simulation cell size. In order to predict the long term effects of irradiation on the material properties of Tungsten, we require a continuum approach to simulate the interactions of dislocation loops in Tungsten due to irradiation. Contemporary continuum models of stress fields from dislocation loops are tricky to handle due to the presence of singularities near the core of the dislocations. We discuss a model which tackles this issue, while producing accurate predictions for the far-field interactions between loops. Such models must be informed by lower length scale simulations so that the physics of the problem is correctly captured by the model, therefore verification via atomistic simulations is important to perform. We compare the current model against predictions produced by atomistic simulations, particularly how the decay rate of atomic displacements scale in the continuum and atomistic simulations, and the handling of finite size effects from the atomistic results.

1.21: Non-Equilibrium Dynamics of 24,000 Electrons Using Real-Space Multigrids: Implementation, Benchmarking, and Stability

Monday, 9:30am, Breakeout 1

Jacek Jakowski,,‡ Wenchang Lu,§ Emil Briggs,§ Liangbo Liang,‡ Panchapakesan Ganesh,‡ and Jerzy Bernholc§

‡ Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA § Department of Physics, North Carolina State University, Raleigh, NC 27695, USA E-mail: jakowskij@ornl.gov

Submitted by:*Jacek Jakowski; jakowskij@ornl.gov; ORNL*

Real-time time-dependent density functional theory (rt-TDDFT) provides a first-principles framework for studying electron dynamics driven by ultrafast fields, relevant to quantum devices, photoactive materials, and plasmonic nanostructures. Despite significant progress, large-scale first-principles simulations of non-equilibrium electron dynamics in extended systems remain computationally challenging due to the need for unitary propagation and long-time numerical stability.

We present the development and implementation of a massively parallel rt-TDDFT module within the open-source Real-space MultiGrid (RMG) code, enabling simulations of electronic dynamics in systems containing up to 24,000 active electrons.[1,2] The formalism employs a density-matrix representation of the Liouville–von Neumann equation, propagated using Magnus expansions to preserve unitarity and energy conservation. The real-space multigrid approach ensures excellent scaling on leadership-class computers.[3]

Benchmarking shows excellent agreement with established TDDFT packages and robust time-integration stability, enabling long-term simulations and excellent conservation of energy over picosecond timescales. We demonstrate applications across a range of systems, from small organic molecules to large plasmonic nanoparticles and field-driven nanostructures. The framework lays the foundation for extensions to spin and nuclear dynamics, offering a general platform for nonequilibrium electronic-structure simulations in complex quantum materials.

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calculations and modeling of materials and molecules. (2024); https://github.com/RMGDFT/

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1.22: Stochastic Coherent State Path Integral approach to Electrons in a Solid

Thursday, 10:40am, Breakout 1

Ingvars Vitenburgs, Jarvist Moore Frost

Submitted by:*Ingvars Vitenburgs; i.vitenburgs23@imperial.ac.uk; Imperial College London*

We develop a stochastic coherent state path integral approach for modeling finite-temperature systems. This is constructed so we can directly sample both Fermion and Boson operator eigenvalues, from any second quantised Hamiltonian. Standard path integral Monte Carlo techniques, sample eigenvalues of coordinate space operators, making the inclusion of spin physics challenging. In the case of the polaron problem this allows us to study more physical interaction forms, e.g. tight-binding models or quartic electron-phonon coupling. We use a spherical Gaussian basis expansion on a lattice. Further we compare to the closed-form solution of a non-interacting quantum harmonic oscillator with a two-site tight binding model, and find passable agreement. We then construct model Hamiltonians for polarons, and compare to ion-trapping experimental data. As we can simultaneously simulate an interacting hole and electron polaron, we predict exciton energies and lifetimes. These we compare to spectroscopic measurements of K-40 impure Bose-Einstein condensates, and solid state gallium nitride time-resolved photoluminesence. Surprisingly we find that electron-phonon coupling has only a moderate effects 10% – 40% on electron-hole recombination times at physical ranges of system parameters. Temperature and, especially, the underlying electronic structure are determined to have the strongest effect on recombination rate. Our method is in early stages in applicability and validity, we believe this new method, could be useful when wanting to include spin-physics in Path-Integral Monte Carlo.

1.23: Distribution of Charge Centers in Matter from Geometric Phases of Electrons

Friday, 8:40am, Breakout 1

Joyeta Saha, Sujith Nedungattil Subrahmanian, Joydeep Bhattacharjee

Submitted by:*Joyeta Saha; joyeta.saha@niser.ac.in; Homi Bhabha National Institute*

We develop a formalism to partition the total electronic charge in matter, derived from the geometric phases of Bloch states. The first-moment matrices of the position operators along the three Cartesian directions do not commute, preventing a simultaneous definition of well-localized charge centers. To address this issue, we construct correlated hermaphrodite Wannier functions by tracing the evolution of Bloch electrons through the Brillouin zone, whose centers capture real-space charge localization with minimal spread. The resulting charge-center maps directly expose inter- and intra-atomic hybridization, revealing diverse bonding behaviors—from localized covalent to delocalized multi-centered bonds—and provide a unified geometric framework for understanding chemical bonding in molecules and solids. (For details, see: J. Saha, S. N. Subrahmanian, and J. Bhattacharjee, J. Phys. Chem. C 128, 18102–18109 (2024).)

Supported by the Department of Atomic Energy, Government of India.

1.24: Propagation of elastic waves in a material with strain gradient magnetism

Thursday, 10:20am, Breakeout 1

Swarnava Ghosh

Submitted by:*Swarnava Ghosh; ghoshs@ornl.gov; Oak Ridge National Laboratory*

We present a theory of elastic wave propagation in a strain gradient magnetic solid with microstructure. We present expressions of frequencies, wave and group velocities of transverse and longitudinal waves. We will also discuss the conditions of attenuation, zero, and negative group velocity of such waves and the phenomenon of wave freezing.

1.25: Competing Electronic, Magnetic, and Volumetric Effects on Hydrogen Binding in Mn/Al Austenitic Iron Alloys

Friday, 9:00am, Breakout 1

Bikram Kumar Das, Mauricio Rincón Bonilla, Elena Akhmatskaya

Submitted by:*Bikram Kumar Das; bdas@bcamath.org; Basque Center of Applied Mathematics, Bilbao, Spain*

Hydrogen embrittlement remains a critical challenge for iron-based alloys. It is highly correlated with hydrogen binding mechanism within the alloy. Here, density functional theory calculations are employed to unravel the factors controlling hydrogen binding in Mn/Al-alloyed austenitic Fe with antiferromagnetic double-layer ordering. We show that Al content and distribution in the first nearest neighbor shell dominate hydrogen solution enthalpy (H-SE), as direct Al–H interactions are strongly repulsive. By contrast, Mn enhances binding, lowering H-SE through volumetric effects and reduced antibonding states. At high Al concentrations, the relative Al distribution and local magnetic environment determine distinct H-SE sub-bundles, whereas volumetric effects are significant only for low-Al environments. Electronic analysis confirms that the interplay between Al–H repulsion, Fe/Mn–H bonding, and magnetovolume effects localizes entirely to the first NN shell. These insights clarify the atomic-scale origins of hydrogen binding, guiding the design of Mn/Al austenitic steels with improved resistance to embrittlement.

1.26: Kinetic magnetism in the crossover between the square and triangular lattice Fermi-Hubbard models

Friday, 10:20am, Breakout 2

Darren Pereira and Erich J. Mueller Cornell University

Submitted by:*Darren Pereira; dlp263@cornell.edu; Cornell University*

We calculate the spin correlations that result from the motion of a single dopant in the hard-core Fermi-Hubbard model, as the geometry evolves from a square to a triangular lattice. In particular, we consider the square lattice with an additional hopping along one diagonal, whose strength is continuously varied. We use a high-temperature expansion which expresses the partition function as a sum over closed paths taken by the dopant. We sample thousands of diagrams in the space of closed paths using the quantum Monte Carlo approach of Raghavan and Elser [Phys. Rev. Lett. 75, 4083 (1995)], which is free of finite-size effects and allows us to simulate temperatures as low as T0.3|t|, even in cases where there is a sign problem. For the case of a hole dopant, we find a crossover from kinetic ferromagnetism to kinetic antiferromagnetism as the geometry is tuned from square to triangular, which can be observed in current quantum gas microscopes.

1.27: Asymmetric fluctuations of growth/retreat on the Kardar-Parisi-Zhang-like surface kinetic roughening for steady crystal growth/retreat

Friday, 8:20am, Breakout 2

Dr. Noriko Akutsu

Submitted by:*Dr. Noriko Akutsu; akutsu@riam.kyushu-u.ac.jp; Research Institute for Applied Mechanics, Kyushu University, Japan*

Kinetic roughening diagrams for a two-dimensional (2D) surface in 3D during steady crystal growth/retreat are constructed using the Monte Carlo method with the Metropolis Algorithm on a lattice model. Surface-height-difference (SHD) distribution functions are also calculated. The positive or negative skewness of the SHD distribution function indicates that the Kardar-Parisi-Zhang (KPZ)-like1 or -like2 [1] kinetically roughened surface has bell-shaped or cup-shaped undulations. The bell-shaped or cup-shaped surface undulations are formed by asymmetric fluctuations of growth/retreat and solid-on-solid restrictions on the surface.
 [1] N. Akutsu and Y. Kangawa, Sci. Rep. 15, 34620 (2025)

1.28: SVD-based analysis of time-series data obtained from real-time TDDFT

Wednesday, 9:40am, Breakout 2

Naoki Tani, Satoru S. Kano, Yasunari Zempo

Submitted by:*Naoki Tani; naoki.tani.7x@stu.hosei.ac.jp; Computer and Information Sciences, Hosei University, Japan*

First-principles calculations for optical spectrum prediction are important for the development of optical materials. In particular, time-dependent density functional theory using real-time and real-space technique (real-time TDDFT) is commonly used to calculate the absorption and emission spectra. In real-time TDDFT, first the times-series data of dynamic dipole moment is calculated and then the polarizability is obtained by Fourier transform (FT). While the former calculation is efficient, the latter spectral resolution is directly limited by the number of time-series data, creating a trade-off with computational cost. To overcome this problem, we introduced a data-driven spectral analysis method instead of conventional FT. Dynamic mode decomposition (DMD) uses singular value decomposition (SVD) to find the data-driven basis functions and computes the oscillation frequency and intensity. Thus, DMD enables higher-precision analysis then FT. We successfully applied this approach to real-time TDDFT results across multiple molecules.

1.29: Vibronic coupling constants calculation with Wannier orbitals for cooperative Jahn-Teller effect

Wednesday, 9:20am, Breakout 2

Zhishuo Huang, Veacheslav Vieru, Naoya Iwahara, Samuel Poncé, Liviu Ungur, Liviu F. Chibotaru

Submitted by:*Zhishuo Huang; zhishuohuang@gmail.com; Technische Universität Berlin*

In recent years, collective phenomena of dynamic Jahn-Teller (JT) centers in crystalline materials have attracted increasing attention. In cubic 5d1 double perovskites such as Ba2MgReO6, the presence of dynamic JT has been confirmed by the signature of vibronic energy levels in resonant inelastic x-ray scattering measurements [1]. Moreover, the experimentally reported unconventional quadrupolar orderings in Ba2MgReO6 and magnetic and quadrupolar orderings in Cs2TaCl6 have been explained based on the concept of vibronic ordering. The theoretical description of these cooperative dynamic JT systems requires accurate derivation and analysis of model Hamiltonians because existing first-principles electronic structure calculations cannot address vibronic dynamics. Quantum chemistry calculations for a JT cluster have often been employed to obtain the local JT model, whereas the calculated model depends on the size/shape of the clusters, and the method does not provide electronic and phonon bands. Moreover, the employed approximations for different interactions are not necessarily consistent with each other. To derive a dynamic JT model for crystals using a unified first principles method, we propose a new approach based on Wannier orbitals for the evaluation of vibronic calculations. We perform verifications and validations of our method and converge it with respect to the size of the supercell. We apply this method to Ba2NaOsO6 and find reasonable agreement with the quantum chemistry method and experimental data. This method is consistent with the framework of first-principles calculations for crystal materials and can be automated. [1] F. I. Frontini et al., Phys. Rev. Lett. 133, 036501 (2024).

Dear conference committee, I have to give lecture between 15:00 and 18:00 (CET) on 4th November. I am not available in the morning of 6th November. Thank you for considering my application of oral presentation and taking into consideration of my special circumstances.

1.30: Correlation Between Nanoscale Crystallinity, Density, and Hydration in Nafion Membranes: Experimental and Molecular Dynamics Insights

Monday, 11:20am, Breakout 2

Mateja Jovanović Freudenberg Technology Innovation SE&Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany Institute of Technical Sciences of the Serbian Academy of Sciences and Arts (SASA), K. Mihailova 35/IV, 11000 Belgrade, Serbia Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia

Dr. Nicolas Bernhard, Matthias Baldofski, Dr. Marcin Rybicki Freudenberg Technology Innovation SE&Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany

Dr. Miljan Dašić, Dr. Igor Stanković Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia

Submitted by:*Mateja Jovanović; mateja@ipb.ac.rs; Junior Research Assistant*

Proton Exchange Membrane Fuel Cells (PEMFCs) represent one of the candidate technologies for sustainable energy conversion. Nafion is considered a benchmark polymer membrane material due to its high proton conductivity and mechanical stability. However, its performance is strongly influenced by the degree of hydration and nanoscale ordering within the membrane. Density-hydration relationships in Nafion have been probed experimentally and computationally for decades. In this work, we examine how local structure determine the density properties, which allows us to interpret experimental observations and results from models, as well as their deviations from theoretical predictions. We observed changes in water phase morphology not only on hydration levels, but on structural configurations as well, we have considered amorphous and crystalline systems. Well hydrated membrane, which ensure connected water domains is crucial for fuel cell performance, enabling a pathway for proton transport. Water clustering in Nafion membranes was analyzed using the DBSCAN algorithm, which groups closely packed molecules while distinguishing sparse regions as noise. This approach enabled the identification of arbitrarily shaped water aggregates and reduced the influence of outliers. The analysis revealed a clear structural transition with hydration: at low water content, water molecules form small, isolated clusters with limited connectivity; at moderate hydration, larger clusters emerge and begin to percolate in crystalline systems; and at high hydration, nearly continuous water networks develop, spanning the entire simulation domain. Additionally, we determined how water content

and membrane structure influence the density of the hydrated Nafion membrane. For all levels of hydration, crystalline configurations have higher densities compared to their amorphous counterparts. That occurs because the spatial ordering allows hydrophobic Nafion backbones to pack closely together with water channels following the direction of the backbones. On the other hand, the globulated nature of the water channels in the amorphous configurations hinders the packing of the backbones, resulting in lower density. Voronoi tesselation analysis reveal that crystallinity enhances molecular packing, yielding higher effective density of the polymer matrix compared to the less ordered amorphous structures. Overall, our findings provide a deeper understanding of how structural ordering influences the density, hydration, and mechanical properties of polymer systems. The interplay between crystallinity and hydration has broad implications for the design of functional polymer materials, particularly in applications such as fuel cell membranes, hydrogels, and biomimetic systems. A combination of molecular simulations, structural analysis, and theoretical modeling offers a powerful framework for predicting the material behavior in hydrated environments, hence guiding future experimental and computational studies in this scientific field.

1.31: Deep Learning Solutions for Modeling Microstructure in Materials

Wednesday, 8:40am, Breakout 1

Hossein Salahshoor, Jianfeng Lu, Rayehe Karimi Mahabadi

Submitted by: *(Amir)Hossein Salahshoor; hossein.salahshoor@duke.edu; Duke University*

From an energy minimization perspective, physical systems often represent several equilibrium states which confers a multi-well structure in their energy landscape. This ubiquitously emerges in mechanics and material science and, in turn, renders the resultant variational problems as non-convex. We present a learning-based framework for approximating Young measures that arise from oscillatory minimizing sequences in nonconvex variational problems and PDE-constrained settings. After discussing emergence of Young measures, in this talk, we present our framework for neural network representation of Young measures. We will demonstrate numerical examples to validate our approach. We will further discuss the applications of our framework for nonlinear mechanics and homogenization.

If possible, I would be grateful if you could schedule my talk at times other than Monday and Wednesday afternoon, Tuesday 10-noon and 3-5 PM.

1.32: Harnessing finite-size effects to gauge aging in the 2D Ising model

Friday, 11:00am, Breakout 2

Dustin Warkotsch, Malte Henkel, Wolfhard Janke

Submitted by:*Dustin Warkotsch; warkotsch@itp.uni-leipzig.de; Universität Leipzig*

The relaxation behavior towards equilibrium of the 2D Ising model with nearest-neighbor interactions has been studied with focus on the two-time autocorrelator C(t, s). Finite-size effects affecting the growing magnetic domains lead to the saturation of C(t, s) with a distinct plateau of height $C_{\infty}^{(2)}(s, L)$ scaling algebraically with waiting time s and lattice size L. These scaling relations are used to produce precise estimates for the autocorrelation exponent and dynamical exponent z with deliberately small lattices. Treating smooth domain walls in a similar manner to the lattice boundaries, their effect on C(t, s) can be understood as premature finite-size phenomenon, extending our ansatz to systems not yet in stationarity.

1.33: Effects of nanochannel geometry and surface properties on water permeation: A molecular dynamics study

Friday, 8:40am, Breakeout 2

Alireza Lotfalinezhad Ali Rajabpour

Submitted by:*Alireza Lotfalinezhad; alirezalotfalinezhad1380@gmail.com; M.Sc. Student, Mechanical Engineering, K. N. Toosi University of Technology, Tehran, Iran,*

This research explores the mechanisms of water uptake within carbon based nanochannels through molecular dynamics simulations, emphasizing the influence of channel geometry, thermal conditions, interaction potential parameters, and structural imperfections. Three nanochannel designs cylindrical carbon nanotubes, square graphene channels, and rectangular graphene slit channels are analyzed, each possessing an identical hydraulic diameter. Among these, the rectangular slit configuration exhibits the highest water transport efficiency, attributed to its open structure, enhanced surface accessibility, and diminished interfacial resistance. Simulation results indicate that elevated temperatures markedly enhance water ingress by increasing molecular mobility, reducing viscosity, and promoting diffusion in confined environments. In contrast, at lower temperatures, water uptake remains limited, suggesting that thermal energy is insufficient to surmount the entry barriers. Surface wettability also plays a pivotal role, with hydrophilic interfaces facilitating more rapid infiltration and stronger water surface interactions. The presence of structural defects such as line vacancies and randomly distributed disruptions significantly hinders water flow by increasing resistance, disturbing hydrogen bonding networks, and compromising the continuity of nanotube walls. The severity of this obstruction correlates with defect density and spatial distribution, affecting both flow rate and molecular alignment. Moreover, defect induced asymmetries can lead to localized trapping and altered transport pathways, further reducing overall efficiency. Collectively, these findings highlight the critical roles of nanochannel architecture, temperature, and surface properties in dictating fluid behavior at the nanoscale. The insights gained offer practical guidance for the design and optimization of nanofluidic systems in applications ranging from filtration and sensing to targeted molecular delivery, energy harvesting, and biomedical diagnostics.

1.34: Joint Wannier Centers (JWCs) in Topological insulators: topological transition from the perspective of chemical bonding

Friday, 9:20am, Breakout 1

NABENDU MONDAL, JOYDEEP BHATTACHARJEE

Submitted by:*NABENDU MONDAL; nabendu.mondal@niser.ac.in; HOMI BHABHA NATIONAL INSTITUTE*

Based on the generalisation of geometric phases of Bloch electrons in multiple bands, we have recently proposed a scheme to obtain a spatial map of possible centres of localised orbitals constituted by the occupied states. The map is a collection of joint Wannier centres (JWC) of correlated hermaphrodite Wannier functions simultaneously contributed by electrons with their crystal momenta evolving through sets of linearly independent directions in the BZ. In this work, we present the study of topological transitions from the perspective of chemical bonding represented by the JWCs. We have explored two-dimensional pristine monolayers by the Kane-Mele model to pinpoint spatially resolved transition thresholds as a function of the distribution of JWCs. Evolution of JWCs has also been investigated from first principles in hydrogenated Xene and traditional bulk TI systems, where the emergence of inter-layer JWCs marks the onset of the TI phase.

1.35: Non-equilibrium steady-state dynamics in the Coulomb glass model

Friday, 9:20am, Breakout 2

Preeti Bhandari, Vikas Malik, and Moshe Schechter

Submitted by:*Preeti Bhandari; preetibhandari15@sau.int; Department of Physics, Faculty of Physical Sciences, South Asian University, New Delhi, India*

We consider here the relaxation properties of Coulomb glass, a system in which all electron states are localized and dynamics occur through phonon-assisted hopping among these states. We model the system as a lattice of localized states, each with a random energy and interacting through the Coulomb interaction. The presence of disorder and long-range interactions makes the system glassy, resulting in a slow tendency towards equilibrium, aging, and memory effects. In this talk, I will discuss my recent work where we employ a kinetic Monte Carlo simulation framework to investigate the electron transport dynamics in a non-equilibrium steady state (NESS) of the lattice Coulomb Glass model. The NESS is induced through the continuous excitation of single electrons to high-energy states by absorption of photons, followed by system relaxation. In proximity to the Fermi level, the NESS approximately conforms to Fermi-Dirac statistics, manifesting an effective temperature (T_{eff}) that exceeds the system's bath temperature (T). The parameter T_{eff} is influenced by both the bath temperature T and the rate of photon absorption by the system. Our findings suggest that the conductivity within the NESS can still be described by the Efros-Shklovskii law, with an effective temperature of $T_{eff} > T$. Furthermore, the predominance of phononless hopping over phonon-assisted hopping is utilized to elucidate the relevance of the hot electron model to the conductivity of the NESS.

1.36: Molecular Dynamics Study on the Role of Graphene Coating in Mitigating Cavitation- Induced Damage on a Metallic Surface

Friday, 9:00am, Breakeout 2

Hatefi Darestani, Roham; Lotfalinezhad, Alireza; Rajabpour, Ali; Kadivar, Ebrahim

Submitted by:*Roham Hatefi Darestani ; Rohamh3622@gmail.com; Department of Mechanical Engineering, Imam Khomeini International University, Qazvin*

Cavitation and its associated effects, including surface erosion and structural degradation caused by the formation and collapse of vapor bubbles, are among the major challenges in marine and mechanical systems. In this study, the influence of graphene coatings with different layer numbers on cavitation-induced damage of aluminum surfaces was investigated using molecular dynamics (MD) simulations. The dynamic interactions between collapsing nanobubbles, the resulting shock waves, and both coated and uncoated substrates were analyzed in detail. The results revealed that the presence of graphene significantly reduced the magnitude of pressure fluctuations, normal stress, and impact forces on the metallic surface. A single-layer graphene coating substantially decreased local pressure peaks and surface deformation compared with the uncoated model. The double-layer graphene further reduced pressure and normal stress, indicating higher energy absorption and damping capability under compressive loading. However, the shear stress analysis showed an increase in tangential stresses in the double-layer system. This behavior arises from the interlayer slip and partial mismatch of mechanical impedance between the graphene layers, which reflect shear waves and localize energy near the interface. Consequently, these effects lead to a renewed increase in the penetration depth of the metallic substrate despite the lower pressure levels. Overall, graphene coatings considerably mitigate cavitation-induced damage, but the optimal performance is achieved with a single-layer graphene, which maintains a balanced resistance to both normal and shear stresses. These findings highlight the potential of atomically thin graphene coatings for improving cavitation resistance in marine propulsion, hydraulic machinery, and energy systems while emphasizing the role of interlayer mechanics in multilayer configurations.

1.37: Elucidating Nonlinear Optical Behavior in Chalcogenometallates: A DFT Study with Emphasis on Perchalcogenometallates

Friday, 9:40am, Breakeout 1

Fatima GARADI, Chikh Lakhdar BENMESSAOUD,Ahmed Lamine BENKAMRI,Hanifi MEBARKI, Mohamed HALIT

Submitted by:*GARADI Fatima ; f.garadi@lagh-univ.dz ; Laboratory of Materials for the Application and Valorization of Renewable Energies, Amar Telidji University, B.P. 37G, Laghouat 03000*

High-performance nonlinear optical (NLO) crystals are essential for advanced photonic and laser technologies. Among the wide range of explored compounds, chalcogenometallates have emerged as promising candidates owing to their excellent transparency and tunable electronic structures in both the infrared and ultraviolet regions. Nevertheless, their practical use remains limited by certain structural and optical constraints. Perchalcogenometallates, a rising subclass within this family, present distinctive advantages by uniting the favorable characteristics of Group-13 elements and chalcogenides. They combine the high laser-damage resistance and structural versatility of Group-13 frameworks with the strong optical nonlinearity and broad transparency window of chalcogenides. Despite this potential, only a few perchalcogenoborates have been reported so far.In this work, we employ density functional theory (DFT) to systematically investigate a non-centrosymmetric perchalcogenoborate crystal, aiming to assess its suitability for nonlinear optical and second-harmonic generation (SHG) applications. The calculated results confirm that the material exhibits mechanical robustness, a moderate band gap, and pronounced birefringence, all of which satisfy the key prerequisites for efficient SHG performance. These findings highlight perchalcogenoborates as a promising class of next-generation NLO materials with potential for future laser and photonic device integration.

Keywords: Nonlinear optical materials; Perchalcogenoborates; Chalcogenometallates; Density Functional Theory; Second Harmonic Generation; Birefringence.

1.38: Large-scale Materials Modeling Using DFT-FE

Monday, 9:50am, Breakout 1

Sambit Das, Vikram Gavini

Submitted by:*Sambit Das; dsambit@umich.edu; University of Michigan*

Large-scale Kohn-Sham density functional theory (DFT) calculations involving tens of thousands of electrons are critical required in variety of application areas, which include extended defects in metals and semiconductors, aperiodic crystals, biomolecules, and many others. However, the stringent accuracy requirements in DFT needed to compute meaningful material properties, in conjunction with the asymptotic cubic-scaling computational complexity with number of electrons, demand huge computational resources. Thus, these calculations are routinely limited to material systems with at most few thousands of electrons. In this talk, I will present a massively parallel real-space DFT framework (DFT-FE) [1-3], which is based on a local real-space variational formulation of the Kohn-Sham DFT energy functional discretized with higher-order adaptive spectral finite-elements, and handles pseudopotential and all-electron calculations in the same framework. I will present the efficient and scalable numerical algorithms in conjunction with HPC centric implementation strategies for the solution of Kohn-Sham equations, that has enabled computationally efficient, fast and accurate DFT calculations on generic material systems reaching 200,000 electrons. DFT-FE demonstrates an order of magnitude performance advantage over widely used plane-wave codes both in CPU-times and wall-times. Finally, I will discuss a successful large-scale application of DFT-FE to modeling of dislocations in crystalline materials, where we computed the core-energetics of pyramidal dislocations in magnesium and dislocation-solute interaction energies in presence of dilute Yttrium solute alloying. These core energetics serve as critical inputs to phenomenological modeling of ductility in magnesium alloys, but have so far been out of reach using plane-wave DFT codes.

[1] Motamarri, P., Das, S., Rudraraju, S., Ghosh, K., Davydov, D., Gavini, V., DFT-FE: A massively parallel adaptive finite-element code for large-scale density functional theory calculations, Comput. Phys. Commun. 246, 106853 (2020). [2] Das, S., Motamarri, P., Subramanian, V., Rogers, D. M., & Gavini, V., DFT-FE 1.0: A massively parallel hybrid CPU-GPU density functional theory code using finite-element discretization, Comput. Phys. Commun. 280, 108473 (2022). [3] Das, S., Kanungo, B., Subramanian, V., Panigrahi, P., Motamarri, P.,

Rogers, D., Zimmerman, P., and Gavini, V., Large-scale materials modeling at quantum accuracy: Ab initio simulations of quasicrystals and interacting extended defects in metallic alloys, SC 2023. (ACM Gordon Bell prize winner)

1.39: vdW-WanMBD: A Wannier-Based DFT Toolkit for calculating van der Waals Interactions

Thursday, 11:20am, Breakout 1

Diem Thi-Xuan Dang, Dai-Nam Le*, Lilia M. Woods Department of Physics, University of South Florida, Tampa, Florida 33620, USA

Submitted by:*Dai-Nam Le; dainamle@usf.edu; Department of Physics, University of South Florida, Tampa, Florida 33620, USA*

We present a novel, cost-efficient framework, namely vdW-WanMBD, for computing dispersive interactions from first principles [1]. This method leverages a Wannier function representation that integrates seamlessly with density functional theory (DFT), enabling a fully electronic many-body treatment of van der Waals (vdW) forces. The approach accurately captures the complete electronic and optical response of materials and allows for the decomposition of vdW and induction contributions. It also facilitates the analysis of anisotropy and stacking-dependent effects in dispersive interactions. Benchmark calculations for layered materials such as graphite, hexagonal boron nitride (hBN), and molybdenum disulfide (MoS) yield binding energies in excellent agreement with experimental data. Additionally, we outline strategies for extending the computational treatment of dispersion forces, aiming to inspire future experimental investigations into vdW interactions across a wider range of materials, particularly in low-dimensional systems. The vdW-WanMBD package is accessible via GitHub [2].

References: [1] Diem Thi-Xuan Dang, Dai-Nam Le, and Lilia M. Woods, “Dissecting van der Waals interactions with Density Functional Theory Wannier-basis approach” Computer Physics Communications 310, 109525 (2025). [2] https://github.com/Diem-TX-Dang/vdW-MBDWan-code

1.40: Quantum Insights into Stick-Slip Phenomena in Nanoscale Tribology

Thursday, 11:40am, Breakout 1

Dai-Nam Le (1,*), Pablo Rodriguez-Lopez (2), Lilia M. Woods (1) (1) Department of Physics, University of South Florida, Tampa, Florida 33620, USA (2) Area de Electromagnetismo and Grupo Interdisciplinar de Sistemas Complejos (GISC), Universidad Rey Juan Carlos, 28933, Móstoles, Madrid, Spain

Submitted by:*Dai-Nam Le; dainamle@usf.edu; Department of Physics, University of South Florida, Tampa, Florida 33620, USA*

Friction in atomistic systems is commonly described by the classical Prandtl-Tomlinson model, which characterizes the dragging force on a nanoparticle in a periodic potential. This study [1] examines a quantum mechanical extension of the model, where dissipation results from heat transfer to an external bath reservoir. The time evolution of the system is modeled using the Liouville von Neumann equation for the density matrix within the Markov approximation. The kinetic and dissipative properties of the nanoparticle are analyzed to differentiate between classical and quantum mechanical effects. Landau-Zener tunneling is identified as a key mechanism that reduces frictional dissipation relative to classical motion, where such tunneling is absent. The analysis clarifies how velocity, interaction strength, and temperature influence frictional processes and provides guidelines for interpreting experimental data.

Reference: [1] Dai-Nam Le, Pablo Rodriguez-Lopez, and Lilia M. Woods. "Quantum stick-slip motion in nanoscaled friction." arXiv preprint arXiv:2502.14207 (2025).

1.41: Performance of an X-alpha functional in band gap prediction

Friday, 10:00am, Breakeout 1

Omololu Akin-Ojo and Usman Kolawole

Submitted by:*Omololu Akin-Ojo; oakinojo@gmail.com; Department of Physics, University of Ibadan, Nigeria*

Predicting the band gap of compounds efficiently and accurately is important in the rapid search of new materials. Density functional theory (DFT) can be helpful in this respect. However, DFT with typical exchange correlation functionals generally underestimate the band gap. There are functionals such as the hybrid functionals that directly or indirectly attempt to correct the band gap predictions but these are generally more compute intensive. The authors of Ref. [1] introduced an approach of tuning the α parameter of the Slater exchange correlation functional to match different atomic properties. We apply this approach for two particular atomic properties and then investigate the performance of these atom-optimized α parameters in predicting the experimental band gap of materials. This approach is able to reduce the band gap error of the LDA DFT functional from 50% to 30%.

References 1. R. R. Zope and B. I. Dunlap, J. Chem. Theory Comput. vol. 13, p1549 (2005)

1.42: First-Principles Investigation of the Electronic and Vibrational Characteristics of Monolayer WSe2

Friday, 10:20am, Breakout 1

Priyanka Jangra and Dr. Ashsih Kumar Mishra

Submitted by:*Priyanka; priyanka.rs.mst21@iitbhu.ac.in; IIT BHU Varanasi, Uttar Pradesh India*

Atomically thin transition metal dichalcogenides (TMDCs) have gained significant attention in recent years due to their outstanding electronic, optical, thermal, and chemical properties, along with their excellent crystalline quality at the two-dimensional (2D) limit. Their bandgap, which typically lies within 1–2 eV, can be tuned by varying the number of layers, making them highly suitable as low-dimensional semiconductors for advanced valleytronic, spintronic, and optoelectronic technologies. The electronic behavior of TMDCs is highly sensitive to thickness variations, allowing for effective control through layer engineering. In the present study, we employ first-principles density functional theory (DFT) calculations using the QUANTUM ESPRESSO package to examine the electronic band structure and phonon dispersion of monolayer WSe2. The computed band structure along the –M–K– high-symmetry path exhibits a direct bandgap of about 1.79 eV, with both the valence band maximum (VBM) and conduction band minimum (CBM) situated at the K point, where strong spin–orbit coupling (SOC) causes distinct splitting of the valence bands. With increasing layer number, enhanced interlayer coupling shifts the VBM toward the point and lowers the CBM between and K, converting the system into an indirect bandgap semiconductor. The phonon dispersion analysis reveals three acoustic branches (ZA, TA, LA), including a characteristic quadratic flexural ZA mode near the point, along with six optical branches primarily governed by the in-plane E and out-of-plane A vibrations. The absence of imaginary phonon frequencies confirms the dynamical stability of monolayer WSe2, while a small LO–TO splitting suggests weak long-range Coulomb interactions compared to the bulk. Overall, these findings demonstrate how layer control effectively tunes the electronic and vibrational properties of WSe2, emphasizing its promise for future nanoelectronic and optoelectronic applications.

2.1: Universal exotic dynamics in critical mesoscopic systems

Friday, 10:40am, Breakeout 2

Nikolaos G. Fytas, Mauro Bisson, Alexandros Vasilopoulos, Massimo Bernaschi, Massimiliano Fatica, Isidoro González-Adalid Pemartín, and Víctor Martín-Mayor

Submitted by:*Nikolaos Fytas; nikolaos.fytas@essex.ac.uk; University of Essex, UK*

We explicitly demonstrate the universality of critical dynamics through unprecedented large-scale Graphics Processing Units (GPU)-based simulations of two out-of-equilibrium processes, comparing the behavior of spin-1/2 Ising and spin-1 Blume-Capel models on a square lattice. In the first protocol, a completely disordered system is instantaneously brought into contact with a thermal bath at the critical temperature, allowing it to evolve until the coherence length exceeds 1000 lattice spacings. Finite-size effects are negligible due to the mesoscopic scale of the lattice sizes studied, with linear dimensions up to $L = 2^{22}$ and 2^{19} for the Ising and Blume-Capel models, respectively. Our numerical data, and the subsequent analysis, demonstrate a strong dynamic universality between the two models and provide the most precise estimate to date of the dynamic critical exponent for this universality class, $z = 2.1676(1)$. In the second protocol, we corroborate the role of the universal ratio of dynamic and static length scales in achieving an exponential acceleration in the approach to equilibrium just above the critical temperature, through a time-dependent variation of the thermal bath temperature.

2.2: Supervised machine learning of continuous and discontinuous phase transitions

Thursday, 10:00am, Breakout 2

Lev Shchur

Submitted by:*Lev Shchur; levshchur@gmail.com; Landau Institute for Theoretical Physics, Chernogolovka, Russia*

We report on the methods developed for extracting information about second- and first-order phase transitions. The first method, applied to continuous phase transitions, is based on binary classification and finite-dimensional analysis of variations in neural network output data when testing data obtained at a known temperature. The second method, applied to discrete phase transitions, is based on ternary classification and analysis of the probabilities of three phases as functions of energy.

2.3: Comparing the relative efficiency of different parallelisation strategies for Wang-Landau sampling: Case study of high-entropy alloys

Monday, 11:20am, Breakout 1

Hubert J. Naguszewski, Christopher D. Woodgate, David Quigley

Submitted by:*Hubert J. Naguszewski; hubert.naguszewski@warwick.ac.uk; University of Warwick*

Flat histogram methods such as Wang–Landau sampling [1] provide an efficient route for high-throughput calculation of phase diagrams in atomistic and lattice-model systems. Numerous parallelisation schemes have been proposed to improve sampling performance across distributed architectures [2-4]. In this study, these schemes are systematically benchmarked—both in isolation and in combination—to establish best practice for scalable flat-histogram simulations [5]. The schemes examined include energy-domain decomposition with both static sub-domains and a dynamic sub-domain sizing approach which we propose. We also assess the benefit of replica exchange and multiple random walkers per sub-domain to determine which factors most strongly influence parallel efficiency and load balance. The influence of sub-domain overlap is likewise discussed. As an illustrative test case, we implement [6] and apply [7] these strategies to a lattice-based model describing the internal energies of the AlTiCrMo refractory high-entropy superalloy, which is known to crystallographically order into a B2 (CsCl) structure with decreasing temperature. Our results demonstrate the superlinear speedup available from energy domain decomposition, and that implementation of non-uniform energy windows has a greater benefit than adding additional random walkers per window.

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2.4: Polynomial-Time Classical Approximate Optimization of Wishart-Planted Spin Glasses

Thursday, 10:40am, Breakout 2

Taozhi Guo, Adil Gangat

Submitted by: *Taozhi Guo; taozhig@princeton.edu; Princeton University*

Approximate optimization of classical spin glasses on complete graphs is of relevance to combinatorial optimization; the Wishart planted ensemble provides a tunably rugged testbed for this task. We propose and test a meta-heuristic that iterates over optimizations of random subsystems and keeps only subsystem updates that lower the global energy; we implement the subsystem optimizations with tensor-network contraction. The meta-heuristic empirically displays polynomial scaling and stable convergence; subsystem size has very little impact on the achievable optimality gap, but larger subsystem sizes lead to smaller scaling exponents. For system sizes up to N=4096, the algorithm achieves optimality gaps below 3% in the computationally “hard” regime and below 20% in the “easy” regime. The optimality gaps reached in the "hard" regime in polynomial time with our meta-heuristic are only reachable in superpolynomial time with certain other state-of-the-art classical heuristics. Our results demonstrate that subsystem-optimization-based meta-heuristics can sometimes have a scaling advantage over other heuristics for approximate optimization of complete-graph classical spin glasses.

2.5: Phase diagram of the square-lattice Potts model in an external field

Thursday, 11:00am, Breakout 2

Shan-Ho Tsai, L. S. Ferreira, J. A. Plascak, D. P. Landau

Submitted by:*Shan-Ho Tsai; shtsai@uga.edu; University of Georgia*

We use Monte Carlo simulations to study the q-state Potts model with q larger or equal to 5 on a square lattice, in the presence of an external magnetic field that couples to one state. Sampling is done using a hybrid algorithm that combines the single spin flip Metropolis method with Wolf cluster updates. The phase diagram in the temperature and external field plane is obtained in the thermodynamic limit by analyzing the finite-size scaling behavior of the order parameters and universal probability distributions. For positive fields and higher values of q, there is a clear first-order transition line that starts at the zero-field transition point and ends at an isolated critical point, which is in the two-dimensional Ising universality class. As the value of state q decreases, the corresponding critical field also decreases. Our results suggest that the critical field vanishes as q approaches 5 from above. For negative fields, another first-order transition line occurs without any critical or multicritical behavior for q larger or equal to 6. The special case with q=5 has a weak first-order transition at zero field and a line of second-order transitions in the 4-state Potts universality class for negative fields.

2.6: Coarsening dynamics and aging of a two-dimensional Coulomb Glass Model

Friday, 9:40am, Breakout 2

Prof. Vikas Malik, Dr. Preeti Bhandari, Prof. Sanjay Puri

Submitted by:*vikas malik; vikas.malik@mail.jiit.ac.in; Department of Physics and Material Science, Jaypee Institute of Information Technology, Noida 201309, UP, India*

In this talk, I present numerical results from a comprehensive Monte Carlo study in two dimensions of coarsening kinetics in the Coulomb glass (CG) model on a square lattice at zero disorder. In the CG model, the electron-electron interactions are unscreened and electrons are localized on lattice sites. The ground state at half filling has antiferromagnetic ordering for zero disorder and disorder less than the critical disorder. The domain growth laws for the two-dimensional CG model at zero and small disorder are analogous to that in the nearest-neighbor Ising model and random field Ising model respectively. Aging studies show that the CG model in zero disorder exhibits simple aging. At small disorders, the CG system exhibits hyperaging. The ground state of the asymmetric CG (slightly away from half filling) at zero disorder, has checkerboard-like pattern with excess holes distributed uniformly. We find that the evolution morphology is in the same dynamical universality class as the ordering ferromagnet.

2.7: Machine-Learning Study of Phase Transitions in Ising Models with Competing Interactions

Thursday, 11:20am, Breakout 2

Maninder Kaur, Ying Wai Li, Dilina Perera, David P Landau

Submitted by:*Maninder Kaur; Maninder.kaur@uga.edu; University of Georgia*

The Ising model is one of the most important models in statistical physics for understanding phase transitions. While the nearest-neighbor ferromagnetic Ising model has been extensively studied [1, 2], incorporating competing next-nearest-neighbor interactions adds complexity to determining its critical behavior. In this work, we study the two-dimensional Ising model with both nearest and next-nearest-neighbor competing interactions. These interactions create new ground states that do not appear in the model with only nearest-neighbor interactions [3]. We used Monte Carlo simulations to generate uncorrelated spin configurations at many temperatures. The data were analyzed using both principal component analysis (PCA) and a neural network to identify distinct phases and detect critical behavior. The leading principal components correspond to the super- antiferromagnetic order parameters, and both PCA and neural-network analyses gave consistent phase distinctions and transition points. The critical parameters—the critical temperature Tc, and the correlation-length exponent were obtained by combining the machine-learning results with finite-size-scaling analysis. The estimated values of Tc and agree well with known numerical estimates. This shows that machine learning can provide efficient ways to study phase transitions in physical systems. References [1] J. Carrasquilla and R. G. Melko. Machine learning phases of matter. Nature Physics, 13(5):431– 434, 2017. [2] Wenjian Hu, Rajiv R. P. Singh, and Richard T. Scalettar. Discovering phases, phase transitions, and crossovers through unsupervised machine learning: A critical examination. Physical Review E, 95(6):062122, 2017. [3] D. P. Landau. Phase transitions in the ising square lattice with next-nearest-neighbor interac- tions. Physical Review B, 22(2):123–145, 1980.

2.8: Low-energy excitations in spin glasses

Friday, 10:00am, Breakout 2

Mutian Shen, Hamid Khoshbakht, Gerardo Ortiz, Yang-Yu Liu, Zohar Nussinov, Martin Weigel

Submitted by:*Martin Weigel; martin.weigel@physik.tu-chemnitz.de; Chemnitz University of Technology*

We consider the effect of perturbing a single bond on ground states of nearest-neighbor Ising spin glasses, with a Gaussian distribution of the coupling constants, across various two and three-dimensional lattices and regular random graphs. Our results reveal that the ground-states are strikingly susceptible to such changes. Altering the strength of only a single bond beyond a critical threshold value leads to a new ground state that differs from the original one by a droplet of flipped spins whose boundary and volume diverge with the system size – an effect that is reminiscent of the more familiar phenomenon of disorder chaos. These elementary fractal-boundary zero-energy droplets and their composites feature robust characteristics and provide the lowest-energy macroscopic spin-glass excitations. Remarkably, within numerical accuracy, the size of such droplets conforms to a nearly universal power-law distribution with exponents dependent on the spatial dimension of the system. Furthermore, the critical coupling strengths adhere to a stretched Gaussian distribution that is predominantly determined by the local coordination number.

I am unavailable Nov 3 + 4 due to an invited seminar elsewhere.

2.9: Non-universality of aging during phase separation of the two-dimensional long-range Ising model

Thursday, 10:20am, Breakout 2

Fabio Müller (Universität Leipzig, Germany) Henrik Christiansen (NEC Laboratories Europe, Heidelberg, Germany) Wolfhard Janke (Universität Leipzig, Germany)

Submitted by: *Wolfhard Janke; wolfhard.janke@itp.uni-leipzig.de; Institut für Theoretische Physik, Universität Leipzig, Germany*

We investigate the aging properties of the phase-separation kinetics in the paradigmatic two-dimensional conserved Ising model with power-law decaying long-range interactions $\sim r^{-(2+\sigma)}$. By means of large-scale Metropolis Monte Carlo simulations, enabled by our novel algorithm for long-range interacting systems, we investigate deep quenches from $T = \infty$ to a finite temperature well below T_c. For all values of the interaction decay parameter σ physical aging with a power-law decay of the two-time autocorrelation function $C(t, t_w) \sim (t/t_w)^{-\lambda/z}$ is observed. The autocorrelation exponent λ displays a complex dependence on σ: For the corresponding nearest-neighbor model (which is recovered as the $\sigma \to \infty$ limit) a value of $\lambda = 3.500(26)$ is determined. In the long-range regime ($\sigma < 1$) the values of λ are all compatible with $\lambda \approx 4$. In between, where also the *equilibrium* critical exponents show a non-trivial σ dependence, a continuous crossover is visible for $1 \lesssim \sigma \lesssim 2$ with non-universal, σ-dependent values of λ.

3.2: Rigorously computing thousands of vibrational states using tensor network methods

Thursday, 11:00am, Breakout 1

Henrik R. Larsson

Submitted by:*Henrik Larsson; larsson@ucmerced.edu; University of California, Merced*

Tensor network states (TNS) have independently advanced the fields of condensed matter physics, electronic structure theory, and vibrational quantum dynamics. Despite their similarities, TNS algorithms applied to electronic and vibrational systems differ substantially, and an in-depth comparison of their strengths and limitations is lacking. In this talk, I will explore the application of the density matrix renormalization group (DMRG) -traditionally used for condensed matter and electronic structure simulations- to vibrational quantum dynamics [1, 2]. I will use the DMRG applied to tree tensor network states to simulate the vibrational spectra of the Zundel ion (HO), the 33-dimensional Eigen ion, and the vibronic spectrum of the NO3 radical, three highly challenging systems characterized by large-amplitude motion and resonances [3, 4]. Finally, I will show that for a widely used benchmark system, TNS algorithms can boost the number of computed states by a factor of five compared to other methods, while simultaneously increasing the accuracy by two orders of magnitude [5]. If time permits, I will show how to directly target excited eigenstates for these systems [6].

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3.3: Many-body theory of positron binding, annihilation and scattering in molecules

Wednesday, 9:00am, Breakout 2

S. K. Gregg and D. G. Green

Submitted by:*Sarah Gregg; s.gregg@qub.ac.uk; Queen's University Belfast*

Positrons are unique probes of matter, with applications in materials science (ultra-sensitive diagnostic studies of surfaces, defects and porosity), medical imaging (positron emission tomography), astrophysics and molecular spectroscopy, and are central to the formation of more complicated antimatter, including positronium and antihydrogen, used for studies of fundamental physics [1].

Low-energy positron interactions with atoms and molecules are characterized by strong many-body correlations, including positron-induced polarization of the molecular electron cloud, screening of the electron-positron Coulomb interaction, and the unique process of virtual-positronium formation (where a molecular electron temporarily tunnels to the positron). They enhance annihilation rates by orders of magnitude, modify scattering cross sections and annihilation gamma spectra, and can enable positron binding. They also make the description of positron-atom/molecule interactions – required to properly interpret fundamental experiments and materials science techniques, and develop antimatter-based technologies – a challenging theoretical and computational problem.

We have developed a diagrammatic many-body theory of positron interactions with molecules which takes ab initio account of key electron-positron correlation effects, implemented in the highly parallelized, Gaussian-orbital-based C++ code, EXCITON+. Our approach provided the first ab initio description of positron-molecule binding in agreement with experiment [2-4], and has accurately predicted positron binding energies for ringed molecules in agreement with new measurements [4]. The many-body framework has also been extended to describe positron annihilation gamma spectra [5], positronic bonding [6] and scattering cross sections [7], with future developments targeting positron interactions in condensed matter. At the conference, I will discuss the computational implementation in EXCITON+ and present new predictions of positron binding energies for substituted ringed molecules composed of C, H, N, O and S atoms [8, 9], which are key components of biologically relevant molecules, highlighting how different substitutions influence positron binding.

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3.4: Applying Tensor Decomposition to Open-Shell CCSD(T)

Monday, 11:40am, Breakout 2

Daniel P. Devore and Devin A. Matthews

Submitted by:*Daniel Devore; ddevore@smu.edu; Southern Methodist University*

Coupled cluster (CC) theory, often regarded as the gold standard of computational quantum chemistry, suffers from a rapid increase in computational cost with molecular size. The computational cost becomes especially prohibitive for large open-shell molecules, which occur in many astrochemical, atmospheric, and biological processes. To address this challenge, we propose the application of Tucker-3 decomposition to approximate the sixth-order excitation tensor t_{ijk}^{abc} as $U_{ai}^{X}U_{bj}^{Y}U_{ck}^{Z}t_{XYZ}$ in the open-shell implementation of coupled cluster theory with single, double, and perturbative triple excitations (UHF-CCSD(T)). This approach effectively replaces the sixth-order tensor with three auxiliary third-order tensors and a compact third-order core tensor. The auxiliary tensors are obtained via the Higher-Order Orthogonal Iteration (HOOI) algorithm, which iteratively applies Singular Value Decomposition (SVD) to a partially compressed triple excitation tensor T_{ck}^{XY} for each spin-case. The Tucker-3 decomposition reduces the overall computational scaling of CCSD(T) from $\mathcal{O}(\mathcal{N}^7)$ to $\mathcal{O}(\mathcal{N}^6)$, where N is the number of molecular orbitals, making the total computational cost comparable to several CCSD iterations.

4.1: Disorder, Dynamics, and Water Confinement in Naphthalene-Diimide Mixed Ionic-Electronic Conductors

Monday, 8:50am, Breakout 2

Marco Severi(1), Filippo Tommaso Garattoni(1), Simiao Yu(2), Chrisitian Nielsen(2), Daniele Fazzi(1)

(1) Department of Chemistry G. Ciamician, University of Bologna, via Piero Gobetti 85,40129 Bologna, Italy (2) Department of Chemistry, Queen Mary University of London, Room 1.08, Joseph Priestley Building, Mile End Road, London E1 4NS

Submitted by:*Marco Severi; marco.severi6@unibo.it; University of Bologna (Italy)*

Organic mixed ionic-electronic conductors (OMIECs) are promising materials for energy-saving and biomimetic applications. These organic conjugated molecules can transport both ionic and electronic charges via coupled conduction mechanisms. Small-molecule OMIECs (e.g., acenes, oligothiophenes, naphthalenediimides) may form amorphous, crystalline, or liquid crystalline phases, which impact device performance. Despite their excellent transport properties and stability, a fundamental understanding of OMIEC structure–function relationships remains limited [1]. To investigate solid-state transport mechanisms, we studied three newly synthesized naphthalenediimide (NDI)-based OMIECs, functionalized with linear alkyl chains (NDI-C10), triethylene glycol chains (NDI-TEG), and crown glycol chains (NDI-crown). Experiments revealed that NDI-C10 and NDI-TEG form crystalline films, while NDI-crown is amorphous. Atomistic molecular dynamics simulations were used to analyse structural and thermal disorder. Accurate force field re-parameterization was crucial to reproduce the experimental crystal structures of NDI-C10 and NDI-TEG. For NDI-crown, we characterized the disordered bulk structure using order parameters and correlation functions drawn from liquid crystal physics [2] and collective behavior studies [3], revealing both global and local dynamic effects relevant to transport. We finally simulated the insertion of water molecules and ions (e.g., NaCl) into the NDI bulk structure, thus elucidating the intercalation effects, the swelling mechanisms and the mass transport properties of the electrolytes in different NDI species. Finally, by quantifying the distinction between confined and bulk water within the materials, we gained insight into water dynamics and structure. These findings contribute to a deeper understanding of OMIECs' structure-dependent transport phenomena, that will lead to design principles for the next generation of devices.

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4.2: All-Atom Reactive Monte Carlo Molecular Dynamics for Molecular Doping in Organic Semiconductors

Monday, 9:50am, Breakout 2

Vishnu Raghuraman, Archana Verma, Nick Jackson

Submitted by: *Vishnu Raghuraman; vishnura@illinois.edu; University of Illinois Urbana-Champaign*

The computational study of molecular doping in organic semiconductors (OSCs) is challenged by multiple competing length and time scales. We present an all-atom Reactive Monte Carlo Molecular Dynamics (RMCMD) method for quantitatively determining molecular doping efficiency in OSCs. A Metropolis criterion is employed for the doping reaction, which is parametrized from density functional theory (DFT) calculations of energetics and atomic partial charges of the doped and neutral molecular species. Polaronic effects are included in the RMCMD method to enable geometric reorganization upon doping, including the flattening of the inter-ring dihedrals. Extensions to partial charge transfer states are also developed to allow for the inclusion of charge transfer complexes. To demonstrate the validity of the approach, the doping efficiency and radial distribution function of a poly(3-hexylthiophene) system doped with 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane are calculated in an amorphous morphology. The method is implemented as a fix in LAMMPS, with the code made publicly available on GitHub.

4.3: Investigating the Role of Solvent Quality on the Nonlinear Rheology of Dynamic Covalent Polymer Networks

Monday, 9:30am, Breakout 2

Muhammed Zeeshan Ahmed and Phillip A. Taylor

Submitted by:*Muhammed Zeeshan Ahmed; ctb8tv@virginia.edu; Department of Chemical Engineering, University of Virginia*

Dynamic covalent polymer networks are reversibly crosslinked soft materials with rapid self-healing, stress relaxation, and tunable viscoelastic properties. Understanding the nonlinear rheology of polymer networks is imperative to designing the next-generation of soft materials for biomedical applications, yet the complex interplay between dynamic covalent bonding and solvent-mediated interactions remains poorly understood. Here, we employ coarse-grained molecular dynamics simulations using a generic bead-spring polymer model to investigate the effect of solvent quality on the nonlinear rheology of dynamic covalent polymer networks comprising 4-arm star polymers under steady (simple) shear. Simulations reveal an increase in viscosity with improved solvent quality, which coincides with a decrease in dynamic covalent crosslink density. Therefore, our simulations suggest that polymer-solvent interactions, rather than polymer-polymer interactions govern the rheological response. Two molecular mechanisms are proposed for the solvent-mediated increase in viscosity: (1) polymer chain bridging via solvent molecules and (2) solvent migration driven by bound solvent on polymer chains. Diffusivity and nearest-neighbor analyses support the latter hypothesis as the dominant mechanism. Overall, our simulations establish molecular-level design rules for tuning the processability and rheology of dynamic covalent polymer networks via solvent quality.

4.4: Micromechanical modeling and numerical evaluation of electrical percolation in carbon nanotube reinforced polymer nanocomposites with homogeneous, agglomerated, and segregated structures

Monday, 8:30am, Breakout 2

Javad Payandehpeyman Mojtaba Mazaheri

Submitted by:*Javad payandehpeyman; j.payandeh@hut.ac.ir; Mechanical Engineering Department Hamedan University of Technology (HUT)*

The electrical performance of carbon nanotube (CNT)/polymer nanocomposites is strongly governed by the morphological characteristics of their internal structures, especially the spatial distribution, waviness, and connectivity of CNT networks within the polymer matrix. Conventional fabrication methods often yield non-uniform dispersions due to the intrinsic length and high aspect ratio of CNTs, promoting particle agglomeration and consequently increasing the electrical percolation threshold. In contrast, recent advances in processing techniques have enabled the formation of segregated network structures that concentrate CNTs at the boundaries of polymer domains, achieving percolation thresholds below 0.01 vol.% and drastically improving electrical conductivity. In this study, a micromechanical model based on mean-field theory is developed to quantitatively capture the influence of agglomeration and segregation on the electrical conductivity and percolation behavior of CNT/polymer nanocomposites. The model represents the composite as a multiphase medium consisting of spheroidal inclusions within a host polymer matrix, allowing differentiation between regions of varying CNT concentrations. By considering the evolution of inclusion volume fractions as a function of total CNT content, the model effectively describes the transformation from homogeneous to agglomerated or segregated morphologies. The theoretical formulation introduces a morphology-dependent parameter, κ, in the percolation relation $P_c = \kappa/M$, where M denotes the CNT aspect ratio. Based on morphology, κ assumes values greater than 0.5 for agglomerated networks, equal to 0.5 for homogeneous structures, and less than 0.5 for segregated morphologies. Model numerical validation was carried out through comprehensive comparisons with published experimental data encompassing a wide range of CNT concentrations and morphologies. The consistency between simulated and measured conductivities confirms the predictive capability of the proposed framework. The results reveal that with increasing CNT aspect ratio, the percolation threshold decreases systematically,

consistent with theoretical expectations.

4.5: Atomistic Origins of Opposite Critical Behavior in Thermoresponsive Ionic Liquid–Water Mixtures: LCST versus UCST

Monday, 9:10am, Breakout 2

Hussen Oumer Mohammed 1,2 Abel de Cozar 1,2,3 Ronen Zangi 1,2,3

1. Donostia International Physics Center(DIPC), 20018 Donostia-San Sebastian, Spain 2. University of the Basque Country (UPV/EHU), 20018 Donostia-San Sebastian, Spain 3. IKERBASQUE, Basque Foundation of Science, 48009 Bilbao, Spain

Submitted by:*Hussen Oumer Mohammed; hussen.oumer@dipc.org; Donostia International Physics Center(DIPC)*

We investigate liquid–liquid phase separation (LLPS) of thermoresponsive ionic liquid (IL)–water mixtures through atomistic molecular dynamics simulations. Two model systems are studied: tetrabutylphosphonium 2,4,6-trimethylbenzenesulfonate, [P4444][TMBS][1], which exhibits a lower critical solution temperature (LCST) phase separation, and protonated betaine bis(trifluoromethylsulfonyl)imid [Hbet][Tf2N], which displays an upper critical solution temperature (UCST) behavior [2]. In both cases, downscaling of the unit ionic charges by a factor of 0.95 was necessary to reproduce the temperature-composition phase diagrams qualitatively. With this model, the spontaneous emergence of the IL-rich and water-rich phases of the biphasic states obtained in the simulations are characterized by compositions that are in excellent agreement with experimental findings. Dynamical properties of these systems, such as viscosities, were slightly retarded (larger by a factor of 2-5) in comparison with experimental values. Aiming to elucidate the driving forces governing the two types of phase separation diagrams, we performed detailed analysis of energy decompositions, hydrogen-bonding networks, and microstructural organizations. We find that for [P4444][TMBS]/water phase demixing, increasing temperature weakens IL–water hydrogen bonds, augments the enthalpic penalty of hydration, and favors ion pairing and mesoscale segregation. Conversely, for [Hbet][Tf2N]/water demixing, cooling enhances water self-networking and suppresses ion hydration, promoting like–like association and apolar domain growth, while heating disrupts the water network and re-establishes miscibility through stronger ion–water hydrogen bonding (anion > cation). By elucidating these molecular-level mechanisms underlying LCST and UCST behavior in distinct ILs, this study offers a predictive, simulation-based framework for the rational design of thermoresponsive draw solutes in forward osmosis

desalination, enabling tunable and energy-efficient regeneration cycles.

Keywords: Ionic liquids, LLPS, LCST, UCST, molecular dynamics, hydrogen bonding, hydrophobic effect, phase diagrams.

Reference

1. Zangi et.al. J. Chem. Inf. Model. 2025, 65, 2, 785–797 2. Zhiping et.al. Environ. Sci. Technol. 2016, 50, 2, 1039–1045

5.1: Insight of the signal transduction in Adenosine A2A receptor by MD simulations

Tuesday, 8:00am, Breakout 2

Duy Phuoc Tran, Akio Kitao

Submitted by:*Duy Phuoc Tran; tpduy@life.isct.ac.jp; School of Life Science and Technology, Institute of Life Science and Technology*

Adenosine A2A receptor is among the receptors in class A GPCR, which strongly be a target of caffein. While the structural biology gives a thorough insight to the static structures of Adenosine A2A receptor in complex with agonists, antagonists, G-protein coupling, there is limited information of how the selectivity types of functional ligands, and cognate and non-cognate G proteins. In this presentation, we would like to introduce our recent efforts to unveil the selectivity of the ligands, and G proteins in coupling to Adenosine A2A receptors through the use of advanced simulation method. While we used to believe the direct binding sites contributing to the activity of the ligands and G-proteins, we found that the allosteric binding sites also exhibit the strong allosteric signal to contribute to the activation of the receptor.

5.2: Incorporation of dose-rate effects into the BIANCA biophysical model and application for space radiation risk assessment

Tuesday, 12:00noon, Breakout 2

E.I. Canay*, M. Carante, A. Casali, E. Bernardini, D. Dondi, Dhanalakshmi Vadivel, L. Cansolino, E. Delgrosso, C. Ferrari, M. Pullia, F. Bonforte, J. Riback, S. Gonzalez, V. Vercesi, F. Ballarini y R. Ramos.

Submitted by:*Ezequiel Ignacio Canay; ecanaycnea@gmail.com; National Atomic Energy Commission (CNEA), Argentina; National University of San Martín (UNSAM), Argentina;*

Space radiation represents one of the main challenges for human exploration beyond Earth's orbit, as it can induce both stochastic and deterministic effects of clinical significance, such as cancer, cataracts, cardiovascular diseases, and neurological damage. During space missions, astronauts are exposed to a chronic low-dose-rate irradiation from galactic cosmic rays (GCR), of the order of 1 mSv/day during solar minimum periods, which may be interrupted by acute high-dose exposures in the case of solar particle events (SPE). In the latter scenario, human organs and tissues may absorb doses of several Gy within a few hours if shielding is insufficient [1]. This particular condition prevents the direct application of radiotherapy models to the space environment, requiring adaptations that account for both sublethal damage repair and the accumulation of lesions over time [2].

In this work, dose-rate effects were incorporated into the biophysical model BIANCA (BIophysical ANalysis of Cell death and chromosome Aberrations) using the Lea-Catcheside formalism [3]. BIANCA is a Monte Carlo-based model that simulates the induction of cell death and chromosome aberrations following photon and heavy-ion irradiations, and has been previously applied to both radiotherapy and space radiation studies [4]. This approach modifies the quadratic term of the linear-quadratic (LQ) model by introducing the so-called "G factor," which allows describing the accumulation and repair of sublethal damage under fractionated or low-dose-rate irradiations. Two repair components were considered: a fast one, with a repair time of 25 min (35% of the total process), and a slow one, with a repair time of 78 min (65%) [5].

The model was validated using experimental cell survival data from both fractionated and acute proton irradiations performed at CNAO (Pavia, Italy) and from the literature. Subsequently, BIANCA was coupled to the FLUKA transport code to simulate the August 1972 solar particle event. RBE-weighted doses were calculated in a voxelized human phantom under different shielding conditions and irradiation durations.

The results show differences of up to 50% between acute and prolonged irradiations in terms of RBE-weighted dose, with this difference decreasing as shielding thickness increases. This highlights the importance of explicitly considering dose-rate effects when estimating the radiobiological risk for astronauts. In conclusion, the extension of the BIANCA model presented in this work improves its predictive capability in space exposure scenarios, enabling a more accurate estimation of RBE-weighted doses during SPEs and providing valuable tools for the planning of future space missions [6].

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5.3: Atomistic Molecular Dynamics Determination of the Fundamental Transverse Mode of B-DNA

Tuesday, 8:20am, Breakout 2

Alireza Masoumi, Ali Rajabpour, Majid Ghadiri, Javad Payandehpeyman

Submitted by:*Alireza Masoumi; a.masoumi@hut.ac.ir; Department of Mechanical Engineering, Hamedan University of Technology, Hamedan, 6516913733, Iran*

We present an atomistic molecular-dynamics (MD) study of the fundamental transverse vibrational mode of a 48-base-pair B-DNA duplex under relevant hydration and ionic conditions. All-atom simulations were performed in LAMMPS using the CHARMM force field, TIP3P water, NaCl ions, and PPPM for long-range electrostatics. A B-DNA, which was immobilized on both terminal segments, was given a controlled transverse displacement, and its center-of-mass (CoM) transverse motion was tracked to extract the modal response. To ensure robustness, we carried out an extensive sensitivity analysis and repeated key runs with three independent random seeds. Energy conservation, reproducibility across seeds, and convergence with respect to numerical parameters were verified. Fourier analysis of the transient CoM trajectory yields a reproducible fundamental transverse frequency in the GHz range for the simulated fragment. The obtained value was validated by Atomic Force Microscopy measurements of DNA dynamics. These findings can be applied to applications in nano-biosensors and gene editing.

5.4: Molecular Dynamic Simulation Study of Deformation Behavior and the Role of Chitosan in Reinforcing Bombyx mori Fibroin Composites Under Acidic Conditions

Tuesday, 8:40am, Breakout 2

Phuc Vu Le, Duy Phuoc Tran, Hanh Thi-Thu Tran

Submitted by:*Le Vu Phuc; vuphucpharma@gmail.com; Ho Chi Minh University of Technology*

Abstract: Despite the demonstrated potential of fibroin and chitosan composites, the precise molecular mechanisms behind their interactions, particularly the interplay between fibroin's hierarchical assembly and chitosan, remain unclear. We employed molecular docking and molecular dynamics simulations to investigate the structure and interactions between chitosan and fibroin. Detailed trajectory analyses, including evaluations of root mean square deviation (RMSD), root mean square fluctuation (RMSF), radius of gyration, and deformation metrics, were conducted to reveal the underlying molecular determinants that govern composite formation. The mechanical properties investigated of the chitosan-fibroin complex reveal potential advantages. The complex exhibits reduced aggregation tendencies, as indicated by greater fluctuations in the radius of gyration, and enhanced fibroin elasticity. By using methodologies from computational physics and materials science, our study aims to bridge the gap between experimental observations and molecular-scale interactions, ultimately guiding the development of advanced fibroin-based composites. These insights hold the promise of informing the design of novel biomaterials with enhanced mechanical, biological, and physicochemical properties, in line with the current thrust toward personalized and regenerative medicine.

5.5: A Fractal Diffusion–Reaction Approach for Modeling Transport and Reactivity in Disordered and Biological Systems

Tuesday, 9:00am, Breakout 2

Neda Valizadeh Gendeshmin, Robabeh Rahimi, Ramin Abolfath

Submitted by:*Neda Valizadeh Gendeshmin; valizadeh.neda1204@gmail.com; Departmentof Physics,UniversityofMoha*
Iran

Understanding how molecular transport and chemical reactions unfold in complex, heterogeneous environments is a central problem that connects physics, chemistry, and biology. Traditional diffusion theories, which rely on assumptions of spatial uniformity, often fail to describe transport in real systems such as disordered solids, porous catalysts, and living tissues. These systems exhibit irregular geometries and limited connectivity that restrict molecular motion, leading to anomalous and scale-dependent diffusion. To address this challenge, we introduce a fractal diffusion–reaction framework that explicitly links the geometry of a medium to its transport and chemical properties, offering a unified perspective on diffusion in non-Euclidean spaces. At the core of this framework is the idea that geometry is not merely a background feature but an active participant in determining dynamical behavior. By formulating diffusion and reaction processes on networks that mimic fractal or self-similar architectures, the model captures how spatial disorder and microstructural complexity regulate the mobility and interaction of reactive species. This approach naturally bridges the microscopic and macroscopic scales, describing how connectivity, tortuosity, and local fluctuations govern the effective transport rates and chemical kinetics of a system. The theoretical model has wide-ranging applications across disciplines. In radiation biophysics, it provides a physical explanation for the FLASH ultra-high dose rate (UHDR) effect, where normal tissues exhibit exceptional resistance to radiation damage while cancerous tissues remain vulnerable. The model attributes this contrast to the underlying structural organization of tissues: the ordered, near-Euclidean architecture of normal tissues enables cooperative diffusion and radical recombination, whereas the fractal disorder of tumors confines reactive species and limits inter-track interactions. Beyond radiobiology, the same framework can describe drug diffusion in heterogeneous tumors, molecular transport in porous materials, charge propagation in amorphous media, and signal transmission in complex biological networks. By integrating fractal geometry directly into the heart of diffusion–reaction theory, this work establishes a versatile and predictive approach to studying transport in disordered environments. It highlights the profound idea that structure governs dynamics-that the shape, connectivity, and scale of a system determine how energy, matter, and information move through it. This perspective not only deepens our understanding of fundamental transport processes but also opens new pathways for designing advanced materials, improving therapeutic strategies, and interpreting the emergent behavior of complex natural systems.

5.6: Metropolis Monte Carlo Simulations in Amino-Acid Sequence Space of Proteins

Tuesday, 9:20am, Breakout 2

Ichiro Takahashi, Takahiro Katagiri, and Yuko Okamoto

Submitted by: *Yuko Okamoto; okamoto@cc.nagoya-u.ac.jp; Nagoya University*

Usual Monte Carlo simulations of protein systems are performed by changing the coordinates of atoms in the proteins. Here, we fix the conformations of proteins and change their amino-acid sequence. We can then examine which amino acids are important for the stability of native protein structures. In this presentation, we give the results of our Monte Carlo simulations of Bovine Pacretic Trypsin Inhibitor which is composed of 58 amino acids.

5.7: Simulation of oxygen diffusion in blood flow

Tuesday, 9:40am, Breakout 2

Tetsuya Yamamoto, Hiroshi Noguchi, Dmitry Fedosov

Submitted by: *Tetsuya Yamamoto; tyamamoto-st@keio.jp; Keio University*

Red blood cells (RBCs) flow through blood vessels to carry oxygen into the microvasculature, where it is released into the blood plasma. The oxygen travels by diffusion and advection, eventually permeating through the vessel walls and further into the tissue. Although there have been extensive studies on oxygen transport on a macroscopic scale, it remains poorly understood at the single-RBC scale. In this study, we explicitly model blood flow including RBCs to numerically investigate oxygen transport in terms of the interactions between RBCs, blood plasma, and vessel walls.

In our simulations, we adopted a mesoscopic model of blood flow based on the smoothed dissipative particle dynamics (SDPD) method. RBCs were constructed by discretizing the cell membrane with bonded SDPD particles. The cytoplasm and the blood plasma were modeled using freely moving SDPD particles, whereas the vessel walls were created by fixing SDPD particles in place. Oxygen diffusion was additionally modeled by solving the diffusion equation between SDPD particles.

In addition to RBC deformation into a parachute-like shape typically seen in capillaries, we observed oxygen diffusion away from the RBCs and into the vessel walls. We found that the oxygen concentration profiles measured using the SDPD model are reproduced well using simplified models solving the advection-diffusion equation in cylindrical coordinates. This suggests that the particulate nature of RBCs can be ignored in certain conditions, lowering computation costs. Furthermore, we observed a nonlinear increase in oxygen retention as the flow velocity was increased.

6.1: The glassy dynamics of multiphase flow: Disorder, frustration and flow regimes

Monday, 10:10am, Breakout 2

Santanu Sinha, Humberto Carmona, Jose S. Andrade Jr. and Alex Hansen

Submitted by:*Santanu Sinha; santanu.sinha@ntnu.no; PoreLab, Department of Physics, Norwegian University of Science and Technology (NTNU), Trondheim, Norway*

Immiscible multiphase flow in porous media in steady state shows different types of flow patterns in different flow regimes, which are described by different pore-scale names such as ganglion dynamics and drop-traffic flow. Here we outline a methodology to analyze the flow patterns in terms of the configurations of the two fluids to characterize the different regimes at the Darcy scale. By considering the pairwise correlations between the two fluids in different pores and maximizing the entropy, we derive a configurational probability distribution with an energy function similar to an Ising spin system. We estimate the coupling constants between the spins in the energy function using inverse Ising model applied to the configurational data from dynamic pore-network simulations. We find the couplings are disordered, with both positive and negative values similar to those in a spin-glass system, and that they follow a Gaussian distribution. Such distribution introduces frustration into the spin-glass system in a certain regime, and we explore its implications in the two-phase flow system. We measure magnetization, the spin-glass order parameter and susceptibilities from the pore-scale configurations to characterize the flow regimes. We point out that here we have considered the steady-state configurations from a dynamic pore-network model, however the method can equally be applied with other computational methods or experimental data.

6.2: Analytical Evaluation of Fin Efficiency Using the Homotopy Analysis Method for Fins with Variable Cross-Section and Temperature-Dependent Thermal Conductivity

Monday, 11:00am, Breakout 2

Amir Basiri Parsa

Submitted by:*Amir Basiri Parsa; amirbparsa@yahoo.com; Assistant Professor, Department of Mechanical Engineering, Hamedan University of Technology, Hamedan, Iran*

Accurate modeling of heat transfer in extended surfaces is essential for optimizing thermal systems, especially when geometric complexity and material nonlinearity are involved. This study presents an analytical approach using the Homotopy Analysis Method (HAM) to evaluate the temperature distribution and efficiency of convective fins with variable cross-sections and temperature-dependent thermal conductivity. The governing nonlinear differential equations are derived from energy conservation principles and solved using HAM, which offers a flexible framework for constructing convergent series solutions without relying on small perturbation parameters. The influence of thermal conductivity variation on fin performance is thoroughly examined, revealing its significant impact on heat dissipation. Comparative analysis with exact solutions confirms the accuracy and robustness of HAM. The study highlights the computational advantages of HAM in solving nonlinear thermal models, aligning with advances in scientific computing algorithms.

7.1: Two-dimensional and three-dimensional Bohm diffusion in N-body plasma simulation

Wednesday, 8:00am, Breakout 2

Yasutaro Nishimura

Submitted by: *Yasutaro Nishimura; nishimura@pssc.ncku.edu.tw; National Cheng Kung University, Taiwan*

An N-body plasma simulation is employed to investigate the Bohm diffusion [1] of electrons in the presence of a uniform background magnetic field. The study examines diffusion in two-dimensions [2,3] (assuming a uniform rod in the magnetic field direction, with the Coulomb force $1/r$ rather than $1/r^2$) and three-dimensions with bouncing boundary conditions. Due to ExB drifts, both cases exhibit D $1/B$ scaling (for 2D, as predicted by Taylor [2]) rather than the $1/B^2$ of the classical scaling. Here, D is the electron diffusion coefficient. If all the charged particles reside on an ideally prepared two-dimensional plane perpendicular to the magnetic field (with the Coulomb force obeying that of 3D), the diffusion process follows the classical scaling. The D values of the latter match the theoretically predicted ones. Numerical methods embedded in the N-body simulation, with an emphasis on binary collisions [5], are briefly recapitulated [6].

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8.1: Diffusion-model approach to flavor physics: A case study for S4’ modular flavor model

Wednesday, 8:20am, Breakout 2

Satsuki Nishimura, Hajime Otsuka, Haruki Uchiyama

Submitted by:*Satsuki Nishimura; nishimura.satsuki.147@s.kyushu-u.ac.jp; Kyushu University*

We propose a numerical method for searching parameters in generic flavor models using a diffusion model, a type of generative artificial intelligence (generative AI). As a specific example, we consider the S4’ modular flavor model and construct a neural network that reproduces quark masses, the CKM matrix, and the Jarlskog invariant by treating the model’s free parameters as generation targets. By generating new parameters with the trained network, we find phenomenologically interesting regions of parameter space that are difficult to explore analytically. Furthermore, we confirm that spontaneous CP violation occurs in the S4’ model. The diffusion model enables an inverse-problem approach, allowing the machine to generate plausible sets of parameters from given experimental constraints. In addition, it can serve as a versatile analytical tool for extracting new physical predictions from flavor models. References are arXiv:2503.21432 [hep-ph] and arXiv:2504.00944 [hep-ph].

8.2: Commercial CMOS imagers for ionizing radiation detection: morphological analysis for particle classification

Wednesday, 8:40am, Breakout 2

María Sol Espain, José Lipovetzky, Martín Alurralde, Martín Pérez, Ezequiel Canay, Sara Josefina González, Agustina Mariana Portu

Submitted by:*Maria Sol Espain; msolespain@gmail.com; National Atomic Energy Commission (CNEA), Buenos Aires, Argentina*

We present an online particle detection technique based on commercial backside-illuminated CMOS image sensors. These sensors provide a compact, low-cost, and modular platform for radiation detection. Their charge collection capability allows direct detection and imaging of the ionization tracks produced by individual particles. Potential applications include ion beam characterization, energy spectroscopy, dosimetry, and boron microdistribution mapping in tissues for Boron Neutron Capture Therapy (BNCT), where it would enable real-time neutron autoradiography with sub-micrometric resolution. A critical technical challenge for these applications is particle discrimination.

In this work we irradiated the sensors with several particle sources at different energies to construct a robust reference database of event clusters. Different machine learning algorithms were trained with this database to enable a reliable classification and precise identification of different particles and energies.

Several commercial, backside-illuminated CMOS camera modules were evaluated. For every irradiation, the protective cover and external optics were removed so that the sensor's active area was directly exposed to radiation. Irradiations were performed with: (i) particles from a 241Am source, with energies tuned from 2 MeV down to 100 keV by varying the source–sensor distance, (ii) rays from a 60Co and 241Am sources, (iii) 7Li ions and protons (p) of several energies (5 Mev - 100 keV) from the Argentine heavy ion electrostatic tandem accelerator (TANDAR).

We extracted a set of 17 morphological and intensity features to evaluate as input for machine learning classifiers. The first analysis shows that the most informative descriptor is the total signal (sum of intensities) of each event. Combined with other 4 additional shape-related metrics, these features separate events generated by particles of different stopping power with high accuracy. A first baseline model (Random Forest) yields promising results in terms of accuracy (85%)

for distinguishing low versus high stopping power events, and we are currently evaluating its performance to classify different particle types.

After various particle irradiations and through rigorous image processing, event segmentation methodology, event exploration and characterization, we have generated a robust and detailed event dataset. Initial tests with simple classifiers already yielded encouraging accuracy, suggesting performance will enhance as the dataset is further improved and the models refined. Particle transport simulations are being conducted in order to verify the energy spectra incident on the sensors and further enhance classification performance.

10.1: Permutation matrix representation quantum Monte Carlo: A universal framework for simulating arbitrary quantum many-body systems

Tuesday, 12:20pm, Breakout 2

Itay Hen, Lev Barash, Nic Ezzell, Arman Babakhani

Submitted by:*Itay Hen; itayhen@isi.edu; University of Southern California*

I will discuss a universal, parameter-free quantum Monte Carlo (QMC) framework capable of simulating arbitrarily structured physical models without the need for model-specific tailoring. The method is based on a generic configuration space and weight formulation that accommodates mixtures of particle types—bosonic, fermionic, or spin systems—and interactions of arbitrary locality, strength, and topology. This generality enables the study of complex quantum many-body systems on arbitrary geometries, from lattice models with higher-order couplings to random systems with long-range or hybrid interactions, all within a single coherent algorithmic architecture. I will demonstrate how this approach unifies disparate QMC flavors under a common formalism and discuss its implications for cross-platform benchmarking, algorithmic extensibility, and the exploration of new classes of Hamiltonians previously inaccessible to traditional QMC schemes.

10.2: Real space formalism for hybrid density functionals

Monday, 10:10am, Breakout 1

Phanish Suryanarayana

Submitted by:*Phanish Suryanarayana; phanish.suryanarayana@ce.gatech.edu; Georgia Institute of Technology*

We present an efficient real space formalism for hybrid exchange-correlation functionals in generalized Kohn–Sham density functional theory (DFT). We implement this formalism for both the unscreened and range-separated variants of hybrid functionals in the SPARC electronic structure code. In particular, we demonstrate up to an order-of-magnitude speedup in time to solution for the real space method. We also develop a modular, math kernel based implementation on NVIDIA architectures, where computationally intensive operations are offloaded to the GPUs, while the remaining workload is handled by the central processing units (CPUs). Considering bulk and slab examples, we demonstrate that GPUs enable up to 8×speedup in node-hours and 80×in core-hours compared to CPU-only execution, reducing the time to solution on V100 GPUs to around 300 s for a metallic system with over 6000 electrons, and significantly reducing the computational resources required for a given wall time.

10.3: Kohn-Sham calculations from one to a million atoms, from ambient conditions to extreme

Monday, 11:00am, Breakout 1

John Pask

Submitted by:*John Pask; pask1@llnl.gov; LLNL*

We discuss algorithms in the open-source SPARC electronic structure code [1] enabling systematically convergent Kohn-Sham calculations of isolated and extended systems, insulating as well as metallic, from one to a million atoms [2], from ambient conditions to a million kelvin [3,4]. Key ideas include high-order discretization on a uniform real-space mesh to enable systematic convergence and computational locality for efficient parallel implementation; local formulation of electrostatics; polynomial filtering for eigenvector refinement in $O(N^3)$-scaling diagonalization based calculations to eliminate longstanding preconditioning bottlenecks; spectral quadrature (SQ) for $O(N)$-scaling density matrix based calculations for large systems and extreme conditions; spectral partition (SP) method for extreme temperatures; and machine learning acceleration. We discuss comparisons to established planewave codes, scaling results for systems of up to a million atoms, and applications to warm- and hot-dense matter at temperatures up to a million kelvin. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. [1] https://github.com/SPARC-X/SPARC. [2] Suryanarayana, Xu, Pask, in Gavini et al., Model. Simul. Mater. Sci. Eng. 31, 063301 (2023). [3] Sadigh, Aberg, Pask, Phys. Rev. E 108, 045204 (2023). [4] Suryanarayana, Bhardwaj, Jing, Kumar, Pask, Phys. Plasmas 32, 033905 (2025).

10.4: Population annealing in the real microcanonical ensemble

Thursday, 11:40am, Breakout 2

Till Pfaff, Denis Gessert, Wolfhard Janke, and Martin Weigel

Submitted by:*Denis Gessert; gessert@itp.uni-leipzig.de; Institute for Theoretical Physics, Leipzig University, Germany*

Population annealing (PA) is an advanced Monte Carlo method aiming at improved sampling in systems with rugged free energy landscape. The canonical form of PA requires sufficient histogram overlap of adjacent annealing temperatures, and therefore is unsuitable for studying first-order phase transitions. To address this limitation, a microcanonical version of PA was proposed [N. Rose and J. Machta, Phys. Rev. E 100, 063304 (2019)], which showed significant improved sampling in the coexistence region. We introduce an adaption of their framework, which shows improved performance. In experiments using the q-state Potts model as our testing ground, we found that the population size required for sufficient equilibration was more than 100 times smaller than in the original formulation. To demonstrate the generality of our method, we consider the first-order region of the Blume-Capel model as a second example. In this second example, annealing in the crystal-field term of the Hamiltonian is necessary, as phase coexistence prevails in the total energy and annealing in the total energy would show little improvement over canonical PA.

11.1: Programmatic Crystal Structure Generation of Catalyst Materials with AI Agents using Fine-Tuned Large Language Models

Tuesday, 12:40am, Breakout 1

Viktoriia Baibakova, Alexey Serov

Submitted by: *Viktoriia Baibakova; baibakovav@ornl.gov; ORNL*

Viktoriia Baibakova1* and Alexey Serov1 1 Energy Storage and Conversion Manufacturing Group, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA *Corresponding author: baibakovav@ornl.gov The rapid discovery of new catalytic materials is constrained by the need for detailed crystallographic inputs and expert-driven workflows. To address this, we present Text2Struc, an AI-driven agent that programmatically generates valid crystal structures from natural-language prompts using a compact large language model (LLM) fine-tuned with Low-Rank Adaptation (LoRA) [1] on a curated text–code–CIF dataset. The fine-tuned model, derived from CodeGen-350M-mono [2], learns to translate textual structure descriptions of varying abstraction into executable code and corresponding crystallographic information files (CIFs). This enables programmatic control of structure generation and manipulation (supercell scaling, strain, vacancy creation, and substitution) via natural-language instructions. Compared to the untuned baseline, fine-tuning reduced hallucination rates from 100% to 5% and improved structural match accuracy up to 82% for fully specified prompts. The model maintained nontrivial inference performance even when only stoichiometry and space group were provided, revealing emergent crystallographic reasoning capabilities. Use cases IrO2, Pb2Ir2O7, NiFe2O4, and Ni3Mo demonstrate the agent's ability to generate physically consistent initial structures suitable for geometry optimization, illustrating applicability to both platinum-group metal catalysts [3] and earth-abundant transition-metal systems [4]. This work establishes a low-energy, language-to-structure pathway that integrates human intent with automated crystallographic reasoning, paving the way for accessible, sustainable, and AI-assisted materials design workflows for catalysts and energy materials. This abstract was authored by c, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy (DOE). The U.S. government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce this manuscript, or allow others to do so, for U.S. government purposes, per the DOE Public Access Plan. [5] References [1] Hu, E.J., Shen, Y., Wallis, P., Allen-Zhu, Z., Li, Y., Wang, S., Wang, L., Chen, W., (2021). Lora: Low-rank

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11.3: Bridging Scales with Continuous-Time Neural Operators for History-Dependent Materials

Friday, 10:40am, Breakout 1

Tanvir Sohail[1], Burigede Liu[2], and Swarnava Ghosh[1] [1]Advanced Computing for Chemistry and Materials Group, National Center for Computational Sciences, Oak Ridge National Laboratory
[2]Department of Engineering, University of Cambridge

Submitted by: *Tanvir Sohail; sohailt@ornl.gov; Oak Ridge National Laboratory*

We present a Continuous-Time Recurrent Neural Operator (RNO) framework for learning and predicting the complex, history-dependent responses of heterogeneous materials across multiple scales. Unlike traditional discrete recurrent networks that depend on fixed time steps, RNO evolves directly in continuous time, eliminating numerical instabilities and reducing computational cost. By learning microscopic spatio-temporal behavior and then upscaling through homogenization, the model efficiently captures the nonlinear and path-dependent features that govern macroscopic material responses. Applied to atomistic-to-continuum simulations and electrohydrodynamic flows, RNO demonstrates remarkable accuracy and robustness, reproducing constitutive behavior while accelerating simulations by several orders of magnitude. This continuous-time neural operator framework establishes a scalable and physics-consistent paradigm for data-driven multiscale modeling in materials science and engineering.

11.4: Learning local and semi-local density functionals from exact exchange-correlation potentials and energies

Tuesday, 9:40am, Breakout 1

Bikash Kanungo, Jeffrey Hatch, Paul M. Zimmerman, Vikram Gavini

Submitted by:*Bikash Kanungo; bikash@umich.edu; University of Michigan*

Finding accurate exchange-correlation (XC) functionals remains the defining challenge in density functional theory (DFT). Despite 40 years of active development, attaining general purpose chemical accuracy is still elusive with existing functionals. We present a data-driven pathway to learn the XC functional by using the exact density, XC energy, and XC potential. While the exact densities are obtained from accurate configuration interaction (CI), the exact XC energies and XC potentials are obtained via inverse DFT calculations on the CI densities. We demonstrate how simple neural network (NN)–based local density approximation (LDA) and generalized gradient approximation (GGA), trained on just five atoms and two molecules, provide remarkable improvement in total energies and densities. Particularly, the NN-based GGA functional attains similar accuracy as the higher rung SCAN meta-GGA on various thermochemistry datasets. These results underscore the promise of using the XC potential in modeling XC functionals and can pave the way for systematic learning of increasingly accurate XC functionals.

11.5: Fast, Modular, and Differentiable Framework for Machine Learning-Enhanced Molecular Simulations

Monday, 11:40am, Breakout 2

Henrik Christiansen, Takashi Maruyama, Federico Errica, Viktor Zaverkin, Makoto Takamoto, Francesco Alesiani

Submitted by:*Henrik Christiansen; henrik.christiansen@neclab.eu; NEC Laboratories Europe*

We present an end-to-end differentiable molecular simulation framework (DIMOS) for molecular dynamics and Monte Carlo simulations. DIMOS easily integrates machine-learning-based interatomic potentials and implements classical force fields including an efficient implementation of particle-mesh Ewald. Thanks to its modularity, both classical and machine-learning-based approaches can be easily combined into a hybrid description of the system (ML/MM). By supporting key molecular dynamics features such as efficient neighborlists and constraint algorithms for larger time steps, the framework makes steps in bridging the gap between hand-optimized simulation engines and the flexibility of a `PyTorch` implementation. We show that due to improved linear instead of quadratic scaling as function of system size DIMOS is able to obtain speed-up factors of up to for classical force field simulations against another fully differentiable simulation framework. The advantage of differentiability is demonstrated by an end-to-end optimization of the proposal distribution in a Markov Chain Monte Carlo simulation based on Hamiltonian Monte Carlo (HMC). Using these optimized simulation parameters a acceleration is observed in comparison to ad-hoc chosen simulation parameters. The code is available at https://github.com/nec-research/DIMOS.

11.6: Machine Learning Excited State Potential Energy Surfaces of Solvated Nile Red with ESTEEM

Wednesday, 9:00am, Breakout 1

Jacob Eller and Nicholas D. M. Hine.

Submitted by:*Jacob Eller; j.eller@warwick.ac.uk; University of Warwick*

Machine Learned Interatomic Potentials (MLIPs) offer a powerful combination of abilities for accelerating theoretical spectroscopy calculations utilising both ensemble sampling and trajectory post-processing for inclusion of vibronic effects, which can be very challenging for traditional ab initio MD approaches [1]. We demonstrate a workflow [2] that enables efficient generation of MLIPs for the solvatochromic dye nile red, in a variety of solvents [3]. We use iterative active learning techniques to make this process as efficient as possible in terms of number and size of DFT calculations [4]. Additionally, we compare the efficacy of various methodologies: generating distinct MLIPs for each adiabatic state, using one ground state MLIP in combination with delta-ML of excitation energies, and using a three-headed multiheaded ML model. To evaluate the validity of the resulting models, we compare predicted absorption and emission spectra to experimental spectra.

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11.7: Shannon Entropy-Based Crystal Structure Prediction of Disordered Alloys via Graph Neural Networks with Alchemical Sampling

Wednesday, 9:40am, Breakout 1

Suman Chabri and Gautam Anand

Submitted by: *Gautam Anand; gautamanand.mst@itbhu.ac.in; School of Materials Science and Technology, Indian Institute of Technology BHU, Varanasi, India*

The prediction of crystal structures in disordered alloys is inherently challenging due to their combinatorial complexity. This complexity grows significantly with the increasing number of atoms, as is typical in high-entropy alloys. Crystal structure prediction for such systems involves two major computational challenges: (i) the development of an efficient atomistic sampling approach and (ii) the establishment of a robust thermodynamic framework for predicting phase stability. In the present investigation, we propose a genetic algorithm–based alchemical sampling approach, referred to as the Genetic Algorithm–Based Atomistic Sampling Protocol (GAASP), to efficiently explore thermodynamically relevant low-energy structures. Alchemical sampling combined with the Metropolis criterion is employed to extensively probe the potential energy landscape of multicomponent, chemically disordered alloys. The sampled potential energy landscape is then used to estimate the phenomenological entropy of different phases. For a given alloy composition, the phenomenological entropy of candidate crystal structures is evaluated, and comparative entropy analysis is employed to predict the most stable single-phase structure. This methodology has been tested on a range of binary, ternary, quaternary, and quinary chemically disordered high-entropy alloys, demonstrating its effectiveness in predicting phase stability in complex alloy systems.

11.8: Machine learning techniques to construct and explore skyrmion phase diagram

Friday, 11:00am, Breakout 1

F. A. Gómez Albarracín

Submitted by:*Flavia A. Gómez Albarracín; albarrac@fisica.unlp.edu.ar; Instituto de Física de Líquidos y Sistemas Biológicos (CONICET - UNLP) La Plata, Argentina*

Undoubtedly, machine learning (ML) techniques have been increasingly used in several physics systems, including condensed matter physics. In the last few years, a number of works have focused on applying ML algorithms to skyrmion textures, topological quasi-particles that are characterized by their robustness and potential technological applications. Here, we present a number of supervised and unsupervised ML approaches to explore different features of skyrmion phase diagrams. First, we introduce a classification technique using a Convolutional Neural Network (CNN) to construct a complete phase diagram from Monte Carlo simulations, focusing on intermediate metastable phases that arise with temperature. Then, we present an unsupervised approach, where we use the anomaly detection technique comparing the reconstruction error of MC snapshots obtained from a convolutional autoencoder trained with parametrised skyrmion lattices, to detect possible exotic phases in skyrmion phase diagrams. Finally, we propose both classification and prediction of skyrmion helicities with a CNN, and apply the trained networks to a whole set of MC simulations to investigate what information may be obtained to build a complete phase diagram.

11.9: A Generalized Framework for Alchemical Machine-Learned Interaction Models in Coarse-Grained Polymer-Grafted Nanoparticle Self-Assembly

Friday, 11:20am, Breakout 2

Melody Y. Zhang*+[1], Shih-Kuang (Alex) Lee*[2], Sharon C. Glotzer[1-3], Rebecca K. Lindsey[1,2]

1Department of Chemical Engineering, University of Michigan 2Department of Material Science & Engineering, University of Michigan 3Biointerfaces Institute, University of Michigan

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Molecular simulations are essential for exploring and optimizing complex colloidal nanoparticle systems, yet they often require a tradeoff between accuracy and computational cost. All-atom simulations provide detailed resolution of interparticle interactions but are prohibitively expensive for large systems. Coarse-grained (CG) approaches overcome this limitation by grouping atoms into an individual interaction site, retaining key chemical features while enabling efficient simulations. However, the high tunability of polymer-grafted nanoparticles (PGNs), namely design parameters such as polymer length and grafting density, makes it challenging to identify optimal conditions for targeted self-assembly. Inverse design strategies address this problem by searching for PGN configurations that yield desired structures, but their success depends critically on accurate descriptions of PGN interactions with respect to inter-PGN distance and the tunable design parameter. Machine-learned interaction models (ML-IAMs) can learn these intricate and higher-dimensional interactions, making them promising tools for describing the interaction landscape for inverse design methods. Here, we present a generalized framework that incorporates a physics-informed “alchemical” dimension into ML-IAMs, enabling continuous mapping between PGN interaction landscapes and tunable molecular design parameters. We integrate steered molecular dynamics (SMD) with the forward–reverse (FR) method[1] into Zhou et al.’s grid sampling strategy[2], allowing efficient generation of potential of mean force (PMF) data for CG PGNs with varying polymer lengths. We use ChIMES[3], a physics-informed ML-IAM, to accurately reproduce PMFs and validate equilibrium structural and thermodynamic properties. We further extend ChIMES into an alchemical model, termed X-ChIMES, which unifies the

PMF landscape across PGN design variables. Finally, by embedding X-ChIMES into the Digital Alchemy framework[4,5], we demonstrate inverse design of PGNs toward target crystal structures and reveal how optimal alchemical parameters shift with self-assembly targets. Our framework provides a broadly applicable strategy for integrating machine learning, coarse-graining, and alchemical design into the discovery of self-assembling nanomaterials.

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12.1: V2Se2O and Janus V2SeTeO: Monolayer altermagnets for the thermoelectric recovery of low-temperature waste heat

Tuesday, 12:20pm, Breakout 1

Shubham Rakesh Singh, Paresh C. Rout, Mohammed Ghadiyali, Udo Schwingenschlögl

Submitted by: *Shubham Rakesh Singh; shubham.singh@kaust.edu.sa; KAUST*

We determine the thermoelectric properties of the V2Se2O and Janus V2SeTeO monolayer altermagnets with narrow direct band gaps of 0.74 and 0.26 eV, respectively. Monte Carlo simulations reveal Néel temperatures of 800 K for V2Se2O and 525 K for Janus V2SeTeO. The electrical conductivity is higher for p-type charge carriers than for n-type charge carriers due to lower effective masses. The presence of heavy Te atoms in Janus V2SeTeO results in lower phonon group velocities, higher phonon scattering rates, and higher lattice anharmonicity than in the case of V2Se2O, leading to an almost 19-fold reduction of the lattice thermal conductivity at 300 K. The thermoelectric figure of merit of V2Se2O reaches 0.4 (0.1) and that of Janus V2SeTeO reaches 2.7 (1.0) just below the Néel temperature at the optimal p-type (n-type) charge carrier density, demonstrating that altermagnets have excellent potential in the thermoelectric recovery of low-temperature waste heat.

Posters

1.101: High-Pressure DFT Study of Lanthanide Monoxides: The B1→B2 Structural Transition

Sergio Ferrari, Daniel Errandonea

Submitted by:*Sergio Ferrari; sergioferrari@cnea.gob.ar; Departamento Física Experimental, CNEA, Centro Atómico Constituyentes, Av. Gral. Paz 1499, San Martín 1650, Argentina;*

We performed a systematic ab initio study of lanthanide monoxides "Ln"O (Ln:La–Lu) under hydrostatic pressure using Density Functional Theory (DFT). At ambient pressure, all compounds are most stable in the B1 (NaCl-type) structure. Upon compression, a pressure-induced B1 → B2 (CsCl-type) structural transition occurs across the whole series, with transition pressures ranging from 29 GPa (YbO) to 209 GPa (LuO). The calculations also provide the equation of state and bulk modulus, which varies smoothly along the lanthanide series (125–152 GPa). These results highlight the relevance of lanthanide monoxides as model systems for understanding high-pressure behavior, with YbO identified as the most suitable candidate for experimental verification.

1.102: Intrinsically patterned 2D transition-metal halides

Neeta Bisht, Andreas Görling, Christian Neiß, Feifei Xiang, Binbin Da, Mohammad Sajjan, Sabine Maier

Submitted by:*Neeta Bisht; neeta.bisht@fau.de; Friedrich Alexander University*

In the quest for complex structured functional materials, defect engineering and patterning in two-dimensional (2D) systems are critical for tuning material properties and enabling new functionalities. Herein, we report on intrinsically patterned 2D transition metal dihalides (TMDs) on a gold surface, featuring periodic halogen vacancies in the upper and bottom halide layers that result in alternating coordination of the transition metal atoms throughout the film.

Employing Density-Functional Theory (DFT) through the Vienna Ab-initio Simulation Package (VASP), we explore the formation pathways leading to periodic halogen vacancies and their role in modifying the electronic and magnetic structure of TMDs. The defect-engineered vacancy lattice not only stabilizes the structure but also provides atomic-level control over the material's properties. Our calculations, enhanced by VASP's robust handling of non-collinear magnetic textures and its accurate simulation of magnetic anisotropy energies, show that Br vacancies are energetically favorable, and the resulting vacancy lattice significantly reduces the lattice mismatch with the underlying Au(111) surface. The structure formation of the 2D FeBr2 on the surface and the presence of defects are further analyzed using STM simulations. The excellent match between the experimental findings and the DFT calculations, facilitated by VASP, confirms the intrinsic vacancy lattice. The electronic band structure accurately captures the Br and Fe contributions in both the pristine and halogen vacancy lattices.

Moreover, our spin-polarized DFT calculations predict the emergence of unconventional magnetic textures, driven by the interplay of defect-induced strain and transition metal coordination. The calculated magnetic anisotropy energy for pristine FeBr2 favors an out-of-plane orientation, while the introduction of vacancies shifts the preferred magnetization to an in-plane direction, demonstrating that vacancies can tune the magnetic properties of the films. By coupling our theoretical results with experimental observations, we provide a comprehensive framework for understanding the structure formation, and electronic and magnetic properties of 2D materials, advancing the design of complex structured materials with tunable properties.

1.103: THE TRANSFORMATIVE EFFECTS OF HYDROGENATION ON THE PROPERTIES OF GERMANENE

Pham Van Luc, Nguyen Minh Phi, Tran Thi Thu Hanh

Submitted by:*Pham Van Luc; mrluc79@gmail.com; Vietnam Atomic Energy Institute (VINATOM); Nguyen Trung Truc High School*

The hydrogenation of the two-dimensional Ge system is studied based on density functional theory. Hydrogen atoms adsorbed onto the two-dimensional Ge surface were recorded to exist at the high warp peak (T1), and the low warp peak (T2) positions. Model optimization is obtained at point k with (5x5x1) MP. When releasing all hydrogen onto the T1 and T2 peak positions, the adsorption energies of all system are calculated. The adsorption site T2 is shown to be the site with the least stable binding ability and the easiest to escape from the 2D Ge surface.

1.104: Distribution of Charge Centers in Matter from Geometric Phases of Electrons

Joyeta Saha, Sujith Nedungattil Subrahmanian, Joydeep Bhattacharjee

Submitted by:*Joyeta Saha; imjoyeta184@gmail.com; Homi Bhabha National Institute*

We develop a formalism to partition the total electronic charge in matter, derived from the geometric phases of Bloch states. The first-moment matrices of the position operators along the three Cartesian directions do not commute, preventing a simultaneous definition of well-localized charge centers. To address this issue, we construct correlated hermaphrodite Wannier functions by tracing the evolution of Bloch electrons through the Brillouin zone, whose centers capture real-space charge localization with minimal spread. The resulting charge-center maps directly expose inter- and intra-atomic hybridization, revealing diverse bonding behaviors—from localized covalent to delocalized multicentered bonds—and provide a unified geometric framework for understanding chemical bonding in molecules and solids. (For details, see: J. Saha, S. N. Subrahmanian, and J. Bhattacharjee, J. Phys. Chem. C 128, 18102–18109 (2024).)

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1.105: Quantum dot and half-metal due to disruption by topological defects at edge of zigzag graphene nano ribbon

Hemant Lohumi, Joydeep Bhattacharjee

Submitted by:*Hemant Lohumi; hemant.lohumi@niser.ac.in; Homi Bhabha National Institute (HBNI)*

Topological defects in graphene are disruptions in the regular hexagonal lattice structure of carbon atoms. These defects can arise naturally during synthesis or it can be introduced intentionally to modify graphene's characteristics. Defects of our interest occur at the junction of two graphene domains with different lattice orientations, typically composed of a series of pentagon-heptagon pairs. Electronic and magnetic properties of the Zigzag-GNRs can be modified by introducing topological defects. We present a systematic study of the effect of topological defects on the electronic structure and transport properties of graphenic nanostructures, aimed in particular towards active device applications through tailoring of the interplay of charge and spin degrees of freedoms of the pz electrons. Topological defects, when introduced at the edges, prominent localized quantum dot states appear at the transmission gap, originating from the chopping of the edge states in that of the pristine nano-ribbon. Localized states peaked at the defects lead to non-trivial drop of transmission amplitude below Fermi energy. With clustering of defects, the width of transmission dip broadens into a wider spin resolved transmission window leading to half metallic transport. ZGNR with topological defect at edge, as can be induced simply by attaching another patch of graphene, thus result into a half metallic window followed by a spin resolved quantum dot regime as a function of gate bias. Our method is based on Green's Functions computed within the mean field approximation of the Hubbard model within a tight binding basis which we will eventually derive from first principles.

1.106: Resonant inelastic x-ray scattering spectra of the dynamic Jahn-Teller Cu2+ center in CuAl2O4

Takumi Gengo (Graduate School of Engineering, Chiba University, Japan) Kenta Touge (Department of Materials Science, Faculty of Engineering, Chiba University, Japan) Ara Go (Department of Physics, Chonnam National University, South Korea) Naoya Iwahara (Graduate School of Engineering, Chiba University, Japan)

Submitted by: *Takumi Gengo; 25wm2218@student.gs.chiba-u.jp; Graduate School of Engineering, Chiba University, Japan*

Cu spinel compounds such as CuAl2O4 [1] and CuGa2O4 [2] attract attention as spin-orbit entangled magnets. The density mean-field theory calculations show that the spin-orbit coupling on the Cu site suppresses the Jahn-Teller deformation in the ground state, which is consistent with the x-ray diffraction data [3]. On the contrary, recent resonant inelastic x-ray scattering (RIXS) measurement of CuAl2O4 suggests the possibility that the Jahn-Teller deformation develops [4]. Such a contradictory situation could occur due to the development of the dynamic Jahn-Teller effect [5]. This study aims to theoretically reveal the nature of the quantum states on Cu sites induced by the competition between the spin-orbit and electron-phonon (vibronic) couplings. We successfully reproduced the Cu L2- and L3-edge RIXS spectra based on our model with the quantum mechanical treatment of the lattice degrees of freedom (i.e., dynamic Jahn-Teller effect), which is consistent with the structural data. This study supports the former theoretical prediction that CuAl2O4 is a 3d spin-orbit coupled magnet [3].

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1.107: First-Principles Investigation of the Structural and Electronic Properties of Tetra-Germanene

Nguyen Minh Phi, Tran Thi Thu Hanh

Submitted by:*Nguyen Minh Phi; nmphi.sdh232@hcmut.edu.vn; Ho Chi Minh City University of Technology (HCMUT), Vietnam National University Ho Chi Minh City (VNU-HCM), Vietnam*

The emergence of non-hexagonal two-dimensional materials has opened new directions for tuning structure–property relationships beyond conventional graphene-like lattices. Among these, tetra-germanene, a predicted square-like allotrope of germanene, has remained largely unexplored. In this work, we employed first-principles density functional theory (DFT) to investigate the atomic configuration and electronic nature of tetra-germanene derived from molecular dynamics simulations. Upon relaxation, the structure transformed into a near-square lattice (a = 4.01 Å, b = 4.17 Å) featuring a pronounced buckling height of 2.18 Å and a cohesive energy of 5.14 eV per atom, indicating greater energetic favorability compared with hexagonal germanene. The distorted square-planar Ge–Ge bonds suggest dsp^3-type hybridization and higher atomic coordination, which distinguish this phase from the typical sp^2/sp^3 bonding in the hexagonal structure. Electronic band-structure analysis reveals a metallic nature with no Dirac crossings near the Fermi level, while density-of-states results highlight strong 4d orbital contributions to bonding. These results demonstrate that tetra-germanene combines greater energetic favorability, metallic conductivity, and structural distinctiveness, making it a promising candidate for next-generation two-dimensional materials in tunable electronics and energy-efficient nanoarchitectures.

1.108: THERMO-MECHANICAL PROPERTIES OF 2D MONOLAYER GOLD: A MOLECULAR DYNAMICS STUDY

Huynh Duy Khang, Tran Thi Thu Hanh

Submitted by:*Huynh Duy Khang; khang.huynhduy@hcmut.edu.vn; Ho Chi Minh City University of Technology (HCMUT), VNU-HCM, Ho Chi Minh City, Vietnam*

Following the experimental synthesis of monolayer gold (Kashiwaya et al., 2024), the temperature-dependent structural evolution and tensile response of goldene remain underexplored by simulation. We investigate temperature-driven structural changes and in-plane mechanical behaviour via classical molecular dynamics in LAMMPS using a baseline EAM potential for Au on a self-constructed 2D periodic sheet, with a two-dimensional constraint applied. After equilibration at 300 K, we perform two protocols: a controlled heating ramp and uniaxial tensile tests along the armchair and zigzag directions. Structural order is monitored through the radial distribution function, coordination statistics, and hexatic order, together with thermodynamic observables. The monolayer is stable at room conditions; upon heating, these indicators reveal progressive loss of order, placing the phase-transition temperature within 1800–2000 K. Under small strain, the elastic response is nearly isotropic between armchair and zigzag. This study provides a qualitative thermo-mechanical picture of goldene and a reproducible MD workflow transferable to other monolayer metals.

1.109: Switching Electronic Properties in a 2D CrI/-InSe Heterostructure via Ferroelectric Polarization

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The integration of two dimensional materials, where one component is a ferroelectric semiconductor, offers a unique opportunity to tune the electronic properties of heterostructures through the application of electric fields. In this context, indium triselenide, -InSe, stands out as an intrinsic low-dimensional ferroelectric material due to its switchable polarization both in-plane and out-of-plane, enabling the design of functional interfaces.

Chromium (ii)iodide (CrI), on the other hand, is a transition-metal dihalide that exhibits ferromagnetic order in its equilibrium structure, with magnetic moments close to 4 B per Cr atom. The lattice parameters of CrI are sufficiently compatible with those of -InSe, allowing their integration into heterostructures without inducing significant strain.

In this work, we employ first-principles calculations based on density functional theory (DFT) to explore the structural, electronic, and magnetic properties of a CrI monolayer and its interaction with a ferroelectric monolayer of InSe. We analyse how the strain induced at the interface stabilizes a Néel-type antiferromagnetic configuration, which is absent in the isolated CrI monolayer. We further examine the influence of InSe polarization on magnetism and charge transfer. Our results show that when the ferroelectric polarization of the InSe is reversed, the band alignment of CrI/InSe switches from a straddling (type I) to a staggered (type II) configuration, and the band gap changes from an indirect gap (0.89 eV) to a direct gap (0.65 eV). These findings reveal a polarization switchable band alignment mechanism, positioning the CrI/InSe heterostructure as a promising candidate for optoelectronic applications.

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1.110: Structural study of the α-phase of $Bi_4V_2O_{11}$

Gustavo Daniel Belletti, Angelina Tamagno, Juan Pablo Sánchez, Paola Quaino

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$Bi_4V_2O_{11}$ can be considered as an intrinsically oxygen-deficient material that constitutes the first member of the Aurivillius family, characterized by alternating bismuth-oxygen layers and perovskite-like vanadium-oxygen blocks. The α polymorph is characterized by a highly ordered framework that incorporates regions of localized disorder within its vanadium–oxygen (V–O) layers. Several models have been proposed to describe the crystal structure of the α-phase of $Bi_4V_2O_{11}$, some derived from experimental data through Rietveld refinement and others based on theoretical approaches. Consequently, the precise structure of α-$Bi_4V_2O_{11}$ remains speculative. Such structural ambiguity is a common feature among Aurivillius phases, such as Bi_2WO_6 and δ-Bi_2MoO_6 which exhibit non-trivial structural complexities. In this work, a series of models derived from an experimentally determined configuration is proposed. The α-phase of $Bi_4V_2O_{11}$ was studied using density functional theory (DFT). A series of structures with comparable energy were identified, characterized by an equal number of oxygen vacancies per V–O layer, diverse vanadium and bismuth coordination environments, and significant variations in Bi–O and V–O bond distances. The results from these models were analyzed and compared with literature data, focusing on the simulation of X-ray diffraction patterns to assess their correspondence.

1.111: Electronic and Spin-Texture Signatures Induced by CO, NO, and O Adsorption on the BiSe(0001) Surface

Julián Castro, Verónica Vildosola, Jorge Facio

Submitted by:*Julián Alejandro Castro; juliancastro@integra.cnea.gob.ar; DFMC, GIyA, CAC, CNEA, INN, CONICET, DF-UBA*

We analyze the adsorption of small molecules on the (0001) surface of BiSe using first-principles density functional theory (DFT) calculations. Specifically, we consider CO, NO, and O adsorbed on a BiSe slab comprising five quintuple layers. Although all these molecules interact weakly with the surface, their highest occupied molecular orbital (HOMO) levels appear at distinct characteristic energies relative to the Fermi level of BiSe, reflecting their different reactivities. In particular, the HOMO level of NO lies within the bulk energy gap, favoring direct hybridization with the topological Dirac surface states and modifying their spin–momentum texture. In contrast, the more stable CO and O molecules have their HOMO levels well below the Fermi energy. While both CO and O bonds weaken upon adsorption, CO molecular orbitals hybridize with non-topological Se surface states. These findings provide insight into molecule–surface interactions involving topological states, with potential implications for catalytic applications.

DFMC: Departamento de Física de Materiales y Complejos.

GIyA: Grupo de Investigación y Aplicaciones.

CAC: Centro Atómico Constituyentes.

CNEA: Comisión Nacional de Energía Atómica (Argentina).

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CONICET: Consejo Nacional de Investigaciones Científicas y Técnicas (Argentina).

DF-UBA: Departamento de Física de la Universidad de Buenos Aires.

1.112: Automatically Assigning Thousands of Vibrational Eigenstates

Wolfgang Kern, Henrik Larsson

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Vibrational spectroscopy is a useful method of characterizing and understanding quantum mechanics in different materials. In order to explain and predict observations, we use the vibrations of harmonic and anharmonic oscillators to give us an assignment of normal modes for bands at certain energies. However, experimental observations for certain materials are not fully interpretable by simulations due to degeneracies and Fermi resonances. One prototypical model for simulation is acetonitrile due to its applications and complicated spectrum that includes many Fermi resonances. Methods using tree tensor network states (TTNSs) and density matrix renormalization group (DMRG) have solved the Schrodinger equation for acetonitrile to high accuracy for thousands of eigenstates. However, manual interpretation is difficult due to the numerous and complicated, resonant eigenstates. We present an automated assignment using Hartree product decomposition that can capture the principal and angular momentum quantum numbers for both degenerate and non-degenerate modes, as well as Fermi resonances and couplings in a spreadsheet. The results are comparable to recent efforts for the first 50 energy states, with additional assignments for 1000 more states. This method is promising to help interpret thousands more states and even be applied beyond to more fluxional systems, such as protonated water clusters.

1.113: Response of a Magnetic Nanoparticle System to a Rotating Magnetic Field

Gustavo P. Saracco and Marisa A. Bab

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The magnetic response of an identical magnetic nanoparticles (MNP) system to a rotating external field (RMF) is studied via Monte Carlo simulations. The field of amplitude H0 and frequency w, was applied in the y-z plane rotating clockwise. The energy was modeled by the Stoner-Wolfharth scheme for fixed or random orientations of the anisotropy, and is in contact with a thermal bath at a temperature T. Interparticle dipolar interactions were also considered. In the non interacting system and for low temperature, hysteresis is observed in the z magnetization component Mz for both orientations of the anisotropy axis and only in the y component (My) for the fixed case. Furthermore, the loop areas were estimated, and increased with w for all orientations and components. At higher temperatures the superparamagnetic state is observed, so both the blocking temperatures TB and loop areas were estimated. The values of TB were close from the room temperature TR=300 °K for all components, and the areas decreased with T but they are practically not zero at TB. When dipolar interactions are included a new scenario is revealed. In the low temperature regime, the blocked state is present for both My and Mz in all anisotropies, and extends beyond the interval of amplitudes H0 estimated theoretically for the model without interactions and fixed anisotropy. The loops are displaced with respect to the origin of the magnetization-external field plane. When the temperature is raised, the blocked state extends for a larger range than the model without interactions, and the loop displacement decreases with T. These behaviors could be explained by observing that the average dipolar field per particle produces an effective field –the sum of both dipolar and external field– that is asymmetric with respect to the zero field line at low temperatures, and becomes half-wave symmetric at higher temperatures. This behavior restores the centered character of the loops. In addition, the loop areas show a peak for all orientations of the anisotropy axes in an intermediate range of temperatures. This result can be associated with a dominance of the anisotropy induced by the dipolar field. Finally, by comparing the areas of the loops of the models with and without interactions, it was found that the non interacting model have larger areas at low temperatures

that vanish near the room temperature, unlike the areas of the model with interactions due to the extension of the blocked state.

1.114: Regression models of H-Pt(100) adsorption energy: from DFT to neural network

Nguyen Van Hoa, Phan Thi Huong, Nguyen Tien Dung, Hoang Hai, Tran Thi-Thu Hanh

Submitted by:*Nguyen Van Hoa; nvhoa.sdh2412@hcmut.edu.vn; Ho Chi Minh City University of Technology (HCMUT), Ho Chi Minh City, Vietnam*

The adsorption process of hydrogen on the Pt(100) surface plays a crucial role in the catalytic activity of platinum for hydrogen oxidation. The adsorption energy is chosen as a characteristic descriptor of this process, representing the energy conversion capability of the catalytic material. This study employs DFT calculations as the foundation to investigate how the adsorption energy varies with different hydrogen coverage configurations on the Pt(100) surface. Eighty distinct adsorption configurations were computed and used as regression data for the H–Pt(100) model. Several regression models were examined, including M0, M1, M2, decision tree, and cluster expansion, using regression algorithms such as multiple linear regression (MLR), XGBoost, and Lasso. Among these, the M2 and cluster expansion models provided the most accurate predictions, particularly capturing the energy discontinuity when the number of hydrogen atoms exceeds that of platinum atoms on the surface. These two models confirm that simplifying the Pt(100) surface with adsorbed hydrogen into an Ising-like system is feasible. Moreover, these models can potentially be applied in future molecular dynamics and Monte Carlo simulations.

1.115: A practical computational protocol for photocatalytic chemical reactions beyond ground-state DFT

Mateusz Wlazło, William A Goddard III, Silvio Osella

Submitted by:*Mateusz Wlazło; m.wlazlo@cent.uw.edu.pl; Centre of New Technologies, University of Warsaw*

Theoretical studies of heterogeneous photocatalysts typically discuss band levels alignment obtained by ground-state DFT which does not capture the physics of light-driven processes. Here, we present a new computational protocol in which excited states are explicitly considered in the Gibbs free energy diagrams of prototypical reactions

1.116: Magnetic exchange interactions in spinels AFe2O4 and ACr2O4 (A = Zn, Cd): a comparative DFT study

C.G. Brusasco, L.A. Errico, A.V. Gil Rebaza

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Ferrites (AFeO) and chromites (ACrO) are semiconducting oxides with spinel crystal structure and exhibit diverse magnetic properties, with potential applications in spintronics and magneto-optical systems [1]. We present a theoretical study based on Density Functional Theory (DFT) within GGA and GGA+U, using two methods: pseudopotentials plus plane-wave (PP-PW) and the full-potential linearized augmented plane-wave (FP-LAPW). Our analysis is framed by the discussion of contradictory results reported for CdCrO. Yaresko [2] reports that the exchange coupling (J) between nearest-neighbours changes of sign with U, meanwhile Lal & Pandey [3] attributed this behaviour to the convergence of DFT+U calculations to local energy minima. For CdCrO, our results differ from those reported previously. Furthermore, we found that the PP-PW and FP-LAPW methods produced different dependencies of Ji with U for the CdCrO. Finally, we examined the potential presence of a magnetoelastic effect in these spinel systems.

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1.118: Engineering Topological Superconductivity via Non-uniform Magnetic Textures: A Real-Space Analysis

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Using a real-space computational methods, we investigate the critical role of external magnetic texture in engineering topological superconducting (SC) phases. This approach, essential for analyzing systems lacking translational symmetry, enables us to compare the topological response of an extended s-wave superconductor under two distinct magnetic configurations: (1) a hybrid Fe-based SC/semiconductor/ferromanget (FM) system comprising a $s_{\pm}$-wave superconductor, a semiconductor with spin-orbit coupling, and a uniform ferromagnetic layer, and (2) an Fe-based SC/skyrmion system comprising a $s_{\pm}$-wave superconductor and a periodic skyrmion lattice. Here the intrinsic Dzyaloshinskii–Moriya interaction of the spins gives rise to a skyrmion texture, which effectively plays the role of spin-orbit coupling as well. Bulk Chern number calculations in real space reveals a fundamental qualitative difference: while the uniform FM field produces a standard topological phase diagram, the skyrmion lattice leads to the emergence of an entirely new phase diagram exhibiting higher Chern invariants that are absent in the FM case. To understand the mechanism of this phenomenon, we employ local Chern number analysis. The results clearly demonstrate that, in contrast to the homogeneous response of a FM system, the skyrmion lattice creates a highly inhomogeneous spatial distribution of topological invariant, namey the Chern numnber. This local inhomogeneity, which directly reflects the complex spin structure of the skyrmion, acts as the primary mechanism for the emergence of bulk phases with high topological invariants. Our result demonstrates that nanoscale magnetic texture engineering, beyond simple symmetry breaking, is a powerful tool for controlled design of novel quantum phases and holds the potential to access topological regimes that might be inaccessible via uniform fields. The importance of real-space computational methods for exploring this rich physics is also highlighted.

1.119: Investigating adsorption and diffusion mechanisms of sodium-oxides on N-doped graphene for an efficient sodium-oxygen battery: A DFT study

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Lithium-ion battery (LIB) is becoming increasingly expensive due to the scarcity of lithium metal and is further constrained by the surging global demand for energy storage. Therefore, promising alternatives, metal-air batteries such as the sodium-oxygen battery (SOB), offer high energy density and low operational costs. Nevertheless, their practical application is limited by the struggle to effectively capture, conduct, and facilitate the movement of these discharge products, a challenge closely associated with the cathode materials. Two-dimensional materials, notably nitrogen-doped graphene (NGr), possess unique properties that make them attractive candidates for next-generation cathodes. In this study, density functional theory (DFT) was used to investigate the adsorption and diffusion behaviors of sodium oxides (NaxO2 , where x = 1, 2, 3, and 4) on NGr. The results revealed strong adsorption energies for isolated Na, O2 , and NaxO2 species, ranging from -1.56 to -2.91 eV. These values are sufficient to prevent decomposition of the adsorbates into the electrolyte during electrochemical processes. Additionally, charge density distribution analyses indicate improved electronic interactions between the NaxO2 and NGr, which are essential for efficient charge transfer. The formation of NaxO2 on NGr with low overpotentials (2.9 V) suggests that NGr could improve the electrochemical performance of SOB. Furthermore, the diffusion energy barriers for the stable NaxO2 on NGr are low (0.07–0.26 eV), indicating high diffusion rates and robustness of NGr as a cathode additive, which could significantly enhance ion transport rates. Despite the adsorption of the non-conductive NaxO2 , NGr maintains its conductive properties, as evidenced by a significant increase in electronic states at the Fermi level. Ultimately, our findings suggest that nitrogen-doped graphene is a highly promising cathode additive for the development of efficient next-generation SOB.

1.120: GW/BSE investigation of the electronic and optical properties of strained and unstrained Sr3NF3

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X3BA3 is a new variant of antiperovskite, which has potential usefulness in optoelectronic and solar device applications. To explore this potential, we used density functional theory (DFT), GW approximation (a many-body perturbation theory method), and Bethe-Salpeter Equation (BSE) approaches to investigate the effect of biaxial strain up to 5% on the electronic and optical properties of Sr3NF3 antiperovskite. We found that the unstrained antiperovskite quasiparticle band gap is a direct gap with a value of 2.06 eV, and its isotropic electronic effective mass is 0.409 mo. Upon applying tensile strain, the gap and effective mass decreased by up to 9.5% and 5.9%, respectively. Furthermore, the absorption spectra from BSE calculations show that the first bright exciton peak (optical gap) from tensile-strained Sr3NF3 is redshifted by up to 200 meV, relative to the unstrained material, whereas compressive strain blueshifted the peak. Other optical properties, such as excitonic binding energy, dielectric function, refraction index, and absorption coefficient, were also found to be strain-dependent. Additionally, a screening of Sr3NF3 for its potential as a photovoltaic device shows that its spectroscopically limited maximum efficiency (SLME, a metric for evaluating the photovoltaic performance limit) increased with tensile strain, reaching up to 27%. Overall, our study indicates that strain plays a significant role in tailoring the properties of Sr3NF3 for applications in optoelectronic and solar cells.

Keywords: antiperovskite, SLME, excitonic peak, tensile strain

1.121: Pseudo-Spectral Approaches to Vortex Dynamics in Nematic Superconductors

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The Ginzburg–Landau (GL) theory has proven to be a highly successful framework for describing the phenomenology observed in superconducting materials. Although the theory is static by construction, in the 1960s Schmid proposed a dynamical extension (time-dependent GL, TDGL) [1] that enables the study of time-dependent phenomena such as vortex dynamics and transport. The resulting equations are nonlinear partial differential equations, requiring numerical methods for their solution.

In superconductivity, finite-difference methods are commonly used; however, they suffer from several drawbacks, including numerical dispersion, numerical dissipation, and spurious oscillations in the simulated fields. Moreover, they typically demand substantial computational time and resources for accurate implementation. In our group, we have developed an approach based on pseudo-spectral methods to solve the TDGL equations, leveraging the Geophysical High-Order Suite for Turbulence (GHOST) package [2–3], originally designed for quantum-fluid turbulence, which constitutes a new application in this area. These methods expand the dynamical variables in a finite (albeit large) set of Fourier modes and integrate the temporal evolution of the expansion coefficients. This approach ensures exponential convergence, contrasting with the algebraic convergence of finite-element methods, and eliminates numerical dispersion and diffusion.

The properties of type-II superconductors are primarily governed by the dynamics and configurations of the vortex system. To investigate this, we simulate vortex dynamics in a model with an s-wave superconducting order parameter coupled to an Ising-type nematic order parameter (the spontaneous breaking of rotational symmetry in electronic properties, observed in several iron-based superconductors). This methodology has already been applied to simulate vortices in superconductors with a nematic order parameter [4] and to study vortex–domain-wall interactions [5]. In this work, we present our latest results [6], where we compute the vortex viscosity in the *flux-flow* regime. Our findings indicate that nematicity induces a pronounced anisotropy in the viscosity, dependent on both the vortex core morphology and the resistive anisotropy of the normal state, as well as on the competitive–cooperative interplay between the two orders.

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1.122: Quantum skyrmions in the antiferromagnetic triangular lattice

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Magnetic skyrmions are topological quasiparticles potentially useful for memory and computing devices. Antiferromagnetic (AF) skyrmions present no transverse deflection and render ultrasmall skyrmion sizes, making them suitable candidates for data storage applications. After the discovery of skyrmions with nanometer length scales, several works presented quantum analogues of classical ferromagnetic (F) skyrmions in spin systems. However, studies about quantum analogues of AF skyrmions are still lacking. We explore the phases of the antiferromagnetic quantum spin-1/2 Heisenberg model with Dzyaloshinskii-Moriya interactions on the triangular lattice using the density matrix renormalization group (DMRG) algorithm. We study the magnetization profile, spin structure factor and quantum entanglement of the resulting ground states to characterize the corresponding phases and signal the emergence of quantum AF skyrmions.

2.101: Neural Network and Monte Carlo studies of the Berezinskii–Kosterlitz–Thouless (BKT) phase transition for the two-dimensional (2D) classical XY model on the honeycomb lattice

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We study the Berezinskii–Kosterlitz–Thouless transition of the two-dimensional (2D) XY Model on the honeycomb lattice using both the methods of Neural Network (NN) and Monte Caro (MC) simulations. The NN employed is a simple multilayer perceptron (MLP) consisting of one input layer, one hidden layer of 512 neurons, and one output layer. In addition, instead of considering real spin configurations to train the MLP, two kinds of artificially made configurations are used as the training set. With semi-experimental formulas, the critical temperature obtained from the MLP calculations is given by 0.572(3). Moreover, based on the helicity modulus, the critical temperature determined from the MC simulations is 0.576(4) which agrees well with that computed from MLP. Both values of the critical temperature we calculate deviate significantly from the well-known approximation result 1/sqrt(2). We give a brief explanation for the difference between our results and 1/sqrt(2).

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2.102: From the Schroedinger Equation to Telescope Designing

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In astronomical imaging, certain systems are composed of multiple apertures, such as lenses or mirrors, arranged together to form what is often referred to in the literature as a segmented telescope or a hypertelescope. These optical systems are essential tools for imaging faint and distant objects in deep space. By combining multiple segments, they can effectively simulate the behavior of telescopes with much larger apertures than traditional systems based on a single monolithic lens or mirror. However, as the size of the lens or mirror increases, fundamental limitations arise that severely restrict or even prevent the use of the telescope. These challenges include the fabrication, transportation, and structural integrity of large mirrors or lenses, which may collapse under their own weight. Launching such components into space becomes practically impossible beyond a certain size. Consequently, there is an upper bound on the aperture size, and thus on the resolution, of telescopes based on continuous, monolithic optics. The challenge of arranging apertures in segmented telescope systems has been the subject of extensive research over the years [Golay1971]. The matter has gained renewed attention following the successful deployment of the James Webb Space Telescope [Greenbaum2013], which demonstrated the immense potential of segmented optics. Existing design strategies often involve trade-offs: tightly packed apertures may lead to redundancies that hinder fault detection and unique segment identification [Cassaing2018], while widely spaced configurations suppress intermediate spatial frequencies, degrading image quality [Liu2024].

One physics inspired approach involved a crystal surface roughness mapping onto a telescope phasing mode [Ribak1990]. Here, we now propose another physics inspired approach to aperture layout optimization by modeling the system as a set of interacting particles governed by a nonlinear Schrödinger-like equation. This method systematically produces configurations with optimal frequency uniformity under the given physical constraints, while preserving the non-redundant character of the system.

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2.103: Mixed-wet percolation

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Inspired by the two-phase flow of immiscible fluids in a mixed-wet porous media, the mixed-wet percolation model is developed. A mixed-wet porous media consists of two kinds of grains (say A and B) with different wetting properties, and the pore throats between A and B grains exert zero capillary pressure on the fluid mixture of two-phase flow. The grains are modelled by ordinary site percolation on the primal lattice, whereas bonds represent the pore throats between the grains in the dual lattice. The primal lattice is populated by the sites which are occupied with probability (p) and remain unoccupied with probability ($1-p$). A bond is placed on the dual lattice separating two adjacent occupied-unoccupied sites of the primal lattice. These bonds represent the zero capillary pressure pore throats, through which the fluid mixture can flow easily. We study the cluster properties of the bond clusters in the dual lattice. These bond clusters are made up of perimeter loops connected to other such loops via knots. An extensive Monte Carlo simulation of the above model has been performed on a square lattice and its dual lattice of different sizes L × L, ranging from L = 200 to 2000, with 100000 realisations. Advanced burning algorithms are implemented to determine the cluster properties. There are two critical thresholds in the system: $p_c = 0.40725$ (same as the threshold of next nearest neighbour site percolation) and $1-p_c = 0.59274$ (same as the threshold of site percolation). The randomness observed in the bond cluster in the dual lattice is not independent but borrowed from the randomness of the site clusters on the primal lattice. For $p_c < p < (1p_c)$, further randomness can be introduced to the bond clusters of the network by placing the bonds in the dual lattice with a certain probability (ω). There exists a critical probability ($\omega_c < 1$) for each value of p, where the network percolates for the first time. Consequently, the percolation transition occurring is not a single point in the parameter space of ω and p, but a continuous curve of critical thresholds of $\omega_c(p)$. The value of $\omega_c = 0.9350$ is the minimum at $p = 1/2$. Various geometrical quantities such as cluster size distribution, fractal dimension, probability of finding a bond in the spanning cluster (order parameter) and fluctuation in order parameter are measured, and the finite-size scaling relations are verified. Surprisingly, the universality class of mixed-wet percolation is found to be the same as that of the bond percolation. Since the bond clusters on the dual lattice form perimeter loops of the site clusters on the primal lattice, they are expected to be in the universality class of the hull percolation, but that is not the case. This is because in this problem, the exterior perimeter loops get connected to the interior perimeter loops via knots and form giant percolation clusters, which have the same property as the percolation cluster. More interestingly, not only the perimeter clusters but also the clusters defined by the knots only (clusters of some disconnected sites) also exhibit the same cluster properties and belong to the percolation universality class.

3.101: Solving the Faddeev Integral Equation without Two-Body t-Matrices Using the Padé Approximation Technique

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In this paper, we propose a novel revision of the Faddeev equation for three-body scattering. Instead of using two-body transition matrices obtained from the solution of the Lippmann–Schwinger equation, this revised formulation directly incorporates the two-body interactions. The proposed approach is expected to simplify numerical implementation and significantly reduce the computation time required for solving the integral equations using the Padé approximation technique.

4.101: Nonequilibrium Dynamics of the Helix-Coil-Transition in Polyalanine

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In this work, the nonequilibrium pathways of the collapse of the helix-forming biopolymer polyalanine are investigated. To this end, the full time evolution of the helix-coil transition is simulated using molecular dynamics simulations. At the start of the transition, short 310-helices form, seemingly leading to the molecule becoming more aspherical midway through the collapse. After the completed collapse, the formation of -helices becomes the prevalent ordering mechanism leading to helical bundles, a typical structural motif representative of the equilibrium behavior of longer chains. The dynamics of this transition is quantified in terms of the power-law scaling of two associated relaxation times as a function of chain length.

4.102: Fullerene-Poly(ethylene glycol) Corona Stabilizes Curcumin in Water: Quantitative Insights from Atomistic Molecular Dynamics

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Curcumin has broad bioactivity but is limited by poor solubility and structural instability in water. We use 100 nanosecond atomistic molecular dynamics to probe a covalent fullerene-poly(ethylene glycol)-curcumin core shell conjugate in which the poly(ethylene glycol) chain contains 25 ethylene oxide units (n = 25), designed to reduce solvent exposure and stabilize curcumin under aqueous conditions. The General Amber Force Field 2 (GAFF2) was applied to model the conjugate in GROMACS. Simulations were performed under isothermal isobaric conditions at 310 K and 1 bar, with electrostatics computed by a smooth particle mesh Ewald method. Structural stability and microencapsulation were quantified through root mean square deviation (RMSD), radius of gyration (Rg), solvent accessible surface area (SASA), atom-atom contacts within 0.6 nm, and radial distribution functions (RDF) for curcumin-poly(ethylene glycol), fullerene-poly(ethylene glycol), and curcumin/fullerene-water pairs. Poly(ethylene glycol) forms a pronounced corona within 0.25-1.5 nm around fullerene and curcumin, as indicated by clear radial distribution peaks and persistent local crowding. Relative to a curcumin-poly(ethylene glycol) control, curcumin in the covalent conjugate shows reduced and narrower Rg fluctuations, consistent with fullerene assisted shape stabilization. The SASA of curcumin decreases markedly in the fullerene containing system, confirming diminished solvent access under the corona. With two curcumin molecules present, curcumin-poly(ethylene glycol) contacts increase compared with the single curcumin case, reflecting local packing and stronger engagement by the corona. Together, these simulation results provide quantitative design handles poly(ethylene glycol) chain length and curcumin stoichiometry for optimizing soft matter carrier architectures.

5.101: Mechanism of curcumin interaction and inclusion by two -cyclodextrin rings: an MD study

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This study investigated the molecular stability, inclusion geometry, and interaction pattern of an enol-form CUR encapsulated by two -CD rings using molecular dynamics (MD) simulations. A geometry-optimized CUR–(-CD)2 complex obtained from DFT optimization in ORCA, with -CDs initially positioned at both ends of CUR, was parameterized in AmberTools using the GAFF2 force field for CUR and q4md-CD parameters for -CDs, solvated in water, and subsequently simulated in GROMACS through energy minimization, NVT/NPT equilibration, and 10 ns production runs. Five independent MD replicates were conducted for statistical reliability. The system reached equilibrium around 8 ns with stable RMSD and radius-of-gyration profiles across replicates. Trajectory analysis revealed a consistent configuration observed across replicates, in which one -CD remained near the CUR terminus while the other migrated toward its central region, forming a dimer-like capsule. Hydrogen bonds between CUR and -CD remained sparse but stable, while -CD–water H-bonds remained abundant, confirming host solvation stability. Interaction-energy analysis showed that Lennard-Jones short-range (LJ-SR) interactions between CUR and -CDs greatly exceeded the Coulomb short-range (Coul-SR) terms, indicating van der Waals and hydrophobic forces as dominant stabilizing contributors. The solvent-accessible surface area (SASA) of CUR encapsulated by -CDs significantly decreased compared with that of free CUR, confirming tight and persistent inclusion. These observations collectively indicate a highly stable inclusion complex driven primarily by nonpolar interactions. Overall, two -CD rings cooperatively encapsulate CUR within a compact dimeric capsule that effectively shields it from solvent exposure and maintains structural stability throughout the simulation. These findings provide a molecular foundation for future studies on the controlled release mechanism of CUR from -CD carriers, offering further insights for rational drug-delivery design.

5.102: Analyzing Beta-Cyclodextrin as an effective carrier for the synergy of Curcumin and Piperine in anticancer bioactivity

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Curcumin, an bioactive compound extracted from turmeric, and Piperine, a natural substance found in black pepper, prosess significant bioactivities that positively impact medical state of human body. However, they both suffer from poor bioavailability limiting their potential. Cyclodextrin (CD), preferably Beta-Cyclodextrin (-CD), is expected to enhance their water solubility and bioavailability with its encapsulation. With the ratio of 1:1:2, this study aims to analyze the co-administration of the two biosubstances along the interaction while encapsulated by -CDs. First, we will find the optimized geometry of the complex through ORCA software. Molecular dynamics (MD) simulations are executed by the help of GROMACS software, CHARMM36 forcefield are used to investigate the complex's behavior in a simple aqueous solution with no participation of ionized atoms. 300K and 0 bar are the average temperature and pressure for the equilization phase. We'll then examine the root mean square deviation (RMSD) of the complex during the MD process, which low value indicating stability is more desirable; stable, ideal radius of gyration (Rg) value, number hydrogen bonds, center-of-mass distances, solvent-accessible surface area (SASA), and water/host radial distribution functions would also be preferable.

5.103: Structural prediction of ensitrelvir-resistant mutants of SARS-CoV-2 main protease

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Introduction Ensitrelvir is an anti-COVID-19 drug which exerts its antiviral activity by inhibiting the main protease (Mpro) of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). In antiviral therapy, even a single amino acid substitution can cause drug resistance. Indeed, the M49I mutant has been reported in several studies to confer resistance to ensitrelvir. In this study, we performed molecular dynamics (MD) simulations on SARS-CoV-2 Mpro. We computationally generated Mpro mutants that have been experimentally confirmed to exhibit drug resistance, aiming to elucidate the structural mechanism underlying ensitrelvir resistance caused by amino acid substitutions. Methods Based on the crystal structure of the SARS-CoV-2 Mpro–ensitrelvir complex (PDB ID: 8dz0), we constructed an initial structure and carried out a 1000 ns MD simulation. We computationally generated several artificial mutant Mpro–inhibitor complexes and performed 100 ns MD simulations for each mutant. Structural changes in the protein backbone, catalytic dyad, and inhibitor position were evaluated using the root mean square deviation (RMSD). Mutants showing minimal changes in the entire protein structure and catalytic dyad, but significant shifts in inhibitor position, were considered likely to confer drug resistance. Results and Discussion Comparison between the computationally generated M49I mutant and the experimentally determined M49I–ensitrelvir co-crystal structure (PDB ID: 8dz1) revealed no significant difference in the RMSD of ensitrelvir. These findings suggest that our modeling approach can reasonably reproduce structural changes in Mpro and their effects on inhibitor binding. Further details will be presented at the conference.

5.104: Structural analysis of the zebrafish fhl1 protein focusing on the zinc fingers

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Some muscle diseases such as reducing body myopathy (RBM) and rigid spine syndrome (RSS) are caused by mutations of FHL1 gene. The FHL1 protein encoded by the FHL1 gene consists of four and a half LIM domains. Each LIM domain has two zinc fingers. In zebrafish, a model organism, it has also been reported that mutation in the fhl1 gene causes symptoms of muscle disease. However, it is unknown how mutations of the fhl1 gene affect the conformation of the fhl1 protein. Therefore, we performed molecular dynamics (MD) simulations to clarify the stable structure of wild-type zebrafish fhl1 protein and the dynamics of it. The 3D structure of zebrafish fhl1 protein predicted by AplhaFold2 was used as the initial structure for MD simulation. MD simulations were performed by using GROMACS 2021.5. We used Amber ff99SB-ILDN for protein and ZAFF for the zinc fingers as force fields, and TIP3P for the water model. We performed 1,000 ns simulations at a constant temperature of 300 K and a constant pressure of 1 bar. We analyzed the structural changes of the fhl1 protein, then focused on the four LIM domains. As a result, we found that among the four LIM domains, the RMSD of the LIM4 domain changed the most. We further focused on the zinc fingers. In this presentation, we report on the fluctuations of the zinc fingers.

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5.105: Simulation of the seasonal supply of entomophilous flower mixtures using Monte Carlo studies

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The availability of floral resources in rural landscapes is key to sustaining arthropod populations that perform ecological functions essential to agriculture, such as pollination [1]. In this interdisciplinary work with researchers specialized in agricultural ecology, the aim was to represent the seasonal variations in the floral supply of different species mixtures selected for establishment in non-farmed areas, optimizing the initial sowing proportions to achieve a homogeneous floral supply over time.

Results are presented for four modeled species that are used as forage plants in the Pampas region of Argentina: white clover (Trifolium Repens), red clover (Trifolium Pratense), yellow sweet clover (Melilotus Officinalis) and chicory (Cichorium Intybus). The dynamics of the species were modeled through Monte Carlo simulations and was based on a Cellular Automaton [2], which includes sowing, flowering and propagation due to seed spreading.

The model was parameterized using bibliographic data on the main demographic variables of each species' life cycle (i.e., germination and mortality rates, and numbers of flowers and seeds per plant), considering different scenarios that account for variability in these parameters according to climatic conditions.

The objective was to ensure and optimize the persistence and seasonal flower supply over a period of two years. Simulations begin during winter, when the initial state is created and seeds with specified proportions are sown. Once seeds are placed in cells, they grow until the bloom period. Plants may die at any time, but only after flowering they leave seeds in their original site or in one of the eight adjacent cells. Propagation of species follows probabilistic rules.

In addition, in order to extend the floral presence in the long run, biannual reseedings were simulated. This process benefits species in decline that fall below specific thresholds. This study presents results of an optimal mixture in three different scenarios of propagation and two reseeding scenarios (manual and automatic).

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5.106: Computational estimation of the effects of the S210R mutation on the structure and enzymatic-activity of CYP2B6 using molecular dynamics simulation

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CYP2B6 is an oxidoreductase containing a heme as an active center, catalyze the metabolic reactions with various medicinal molecules, e.g., anti-human immunodeficiency drug, efavirenz (EFZ). Amino acid mutations in CYP2B6 caused by genetic polymorphisms significantly impact on its drug responsiveness, leading to individual differences in drug efficacies. Previously, we experimentally evaluated the functional changes caused by missense mutations in CYP2B6 identified from Japanese individuals and revealed that several mutations including S210R significantly reduced the enzymatic activities of CYP2B6. In this study, the molecular dynamics (MD) simulations were performed on wild-type CYP2B6 and S210R mutant to elucidate the mechanism of the reduction of enzymatic activity caused by S210R mutation. The simulation template was constructed by docking EFZ onto the crystal structure of CYP2B6 (PDB ID: 3IBD). The systems were solvated using TIP3P water molecules in a truncated octahedral box. After the systems were fully relaxed, the 1500-ns MD simulations were performed to equilibrate the entire system. In the equilibrium structure, no substantial difference in the relative position of the EFZ was observed between the wild-type CYP2B6 and S210R mutant. On the other hand, the two highly-frequent hydrogen bonds between Ser294 and EFZ were observed in the wild-type CYP2B6, whereas the occurrence frequencies of the corresponding hydrogen bonds were greatly reduced in the S210R mutant. In addition, the flexibility of the FG region, comprising the substrate-access channel and active site, was higher in the wild-type CYP2B6 than that in the S210R mutant. These can explain the reduction of enzymatic function of the S210R mutant relative to the wild-type CYP2B6.

6.101: Magnetized turbulent combustion

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The deflagration to detonation transition (DDT) is believed to be one of the critical mechanisms in Type Ia supernovae (SNe Ia), enabling the transition from subsonic burning to a detonation wave in a turbulent white dwarf environment. While existing models, such as the data-driven subgrid scale approach by Gusto (2022), focus on the role of turbulence in plasma preconditioning within the Zel'dovich gradient mechanism, the precise energy sources that facilitate this transition remain an open question. A growing body of evidence suggests that localized ignition clusters, regions of hot plasma with short ignition times, play a crucial role in triggering detonation. The survival of these clusters depends on their ability to remain isolated from turbulence and avoid rapid mixing, allowing nuclear burning to accelerate and eventually lead to full ignition. However, the mechanisms that sustain these ignition kernels and supply the necessary energy remain unclear. In this study, we investigate magnetic reconnection as a potential source of energy release that could influence DDT conditions. Magnetic reconnection is a fundamental process in plasmas that involves the rapid conversion of magnetic field energy into plasma thermal energy. This leads to localized heating and turbulence, which may significantly impact hotspot formation and thermonuclear runaway in the pre-detonation phase. To explore this hypothesis, we use the FLASH code to perform a series of computational experiments simulating reconnection driven energy release in burning dense stellar plasmas. Our approach builds on the reconnection analysis techniques of Servidio et al. (2009), which utilize magnetic field topology to identify reconnection regions, and we compare these results with the recently proposed method by Wang et al. (2024). We extend previous reconnection studies by reconstructing full-volume Euler potentials from simulation data to recover divergence free magnetic fields and quantify reconnection rates. To improve the resolution of steep gradients and suppress spurious oscillations in FLASH output, we apply fifth order Weighted Essentially Non-Oscillatory (WENO) reconstruction to key plasma fields prior to reconnection analysis.

7.101: Effect of Magnetic Field on the Formation and Properties of Ion-Acoustic Double Layers in Space Plasmas

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Electrostatic double layers (DLs) are nonlinear potential structures that play a crucial role in the acceleration of charged particles in space plasma environments. In this work, we investigate the influence of an external magnetic field on the formation and stability of ion-acoustic double layers in a multi-component plasma composed of adiabatic ions and two distinct populations of non-Maxwellian electrons. Using the Sagdeev pseudo-potential approach, we analyze how the obliquity and strength of the magnetic field modify the potential well structure and affect the critical Mach numbers associated with DL formation. The results demonstrate that increasing magnetic field strength tends to suppress the amplitude and width of the DL, leading to stronger localization of the potential jump and reduced ion acceleration.

7.102: Influence of Nonextensivity on Current Density and Sheath Structure in Warm Ion Plasmas

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In this study, a plasma composed of nonextensive electrons and singly charged warm positive ions is modeled using hydrodynamic equations. The governing fluid equations are solved numerically to examine how the degree of nonextensivity, represented by the parameter (q), affects the current density and sheath characteristics. The analysis reveals that increasing the (q)-parameter enhances the charged particle current density within the sheath region. It is further observed that the current density at the plasma–sheath interface remains nearly independent of (q), while the sheath thickness decreases with increasing nonextensivity

7.103: On the effect of Electron distribution on Double Layer Formation in Beam-Driven Plasmas

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Electrostatic double layers are key nonlinear structures responsible for particle acceleration and localized potential drops in various plasma environments. In this study, we investigate the formation of double layers in a non-Maxwellian plasma consisting of warm ions, kappa-distributed electrons, and an additional warm electron beam. The Sagdeev pseudopotential approach is employed to analyze the conditions for double layer existence and to evaluate the modified Bohm criterion in such a plasma. The results reveal that while the influence of the beam parameters on the critical Mach number is minimal, the nonthermal characteristics of the background electrons, represented by the kappa index, play a dominant role in determining the threshold and strength of the double layer.

8.101: Thick Target Yield Analysis of Proton-Induced Reactions on Selenium for Theranostic Bromine Radioisotope Based on Machine Learning Results.

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This study investigates the thick target yield (TTY) of proton-induced reactions on selenium for the production of theranostic bromine radioisotopes 76Br and 77Br. While 76Br (half-life 16.2 h) is suitable for PET imaging due to its positron emission and moderate half-life, 77Br (half-life 57.0 h) is a promising candidate for targeted molecular therapy through Auger electron emission. The yield (Y) was calculated using the relation: $Y = (N_A \times H)/(M \times z \times q_e) \times \int[E_{em} \rightarrow E_{inc}](dE/dx)^{-1} \times \sigma(E)dE$, where N_A is Avogadro's number, H is the isotopic enrichment fraction, M is the molar mass of the target isotope, z is the projectile charge, q_e is the elementary charge, (dE/dx) is the stopping power, and $\sigma(E)$ is the reaction cross-section as a function of energy. The integration limits E_{inc} and E_{em} correspond to the incident and emergent proton energies, respectively.

The energy limits were determined for a 1-mm selenium target. The incident energy (Ein) was taken as the proton energy at the cyclotron exit, while the emerging energy (Eout) was obtained by accounting for energy loss through the target, using stopping-power data extracted from SRIM. This approach reproduces realistic experimental conditions and ensures accurate estimation of the effective energy range contributing to the yield.

Cross-section data were obtained from two sources: (1) experimental data reconstructed via machine-learning models from our previous work [1], and (2) theoretical results from the TALYS-2.0 code [2]. While TALYS provides a continuous energy range, its accuracy decreases in resonance regions and for multi-neutron emission channels such as 76Se(p,2n)75Br and 77Se(p,2n)76Br.

Two main reactions were analyzed: 76Se(p,n)76Br and 77Se(p,n)77Br. For 76Br, the dominant impurity is 75Br, produced through the competing 76Se(p,2n)75Br channel above approximately 15–16 MeV. For 77Br, the main impurity is 76Br, formed via the 77Se(p,2n)76Br reaction above about 6–7 MeV. These isotopic impurities are difficult to separate from the desired product by conventional chemical methods.

The maximum yields were approximately 1.33 × 10 MBq/µA at 16–18 MeV for 76Br and about 928 MBq/µA at 6–8 MeV for 77Br. These results define optimal energy ranges for efficient cyclotron production of bromine radioisotopes for imaging and therapeutic applications.

Keywords: Proton-induced reactions; Thick target yield; Selenium; Bromine radioisotopes; Machine learning; TALYS.

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8.102: Autoencoder Latent Representations and One-Dimensional Convolutional Neural Networks for the Identification of Composite Radioisotopes

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Accurate and reliable identification of isotopes from short-duration, low-count -ray spectra is a fundamental requirement for nuclear protection and security as well as environmental monitoring. In operational settings, spectra are typically affected by background and instrumental disturbances; therefore, identification models must provide not only high accuracy but also sufficient stability and reliability. In this work, two approaches are proposed and evaluated for the identification of composite radioisotopes: (i) using an autoencoder latent space with classification by a multilayer perceptron (MLP), and (ii) a one-dimensional convolutional neural network (1D-CNN) that learns spectral features directly from the 1,024-channel input spectrum. Both methods are trained on simulated spectra. These spectra are generated to reflect realistic conditions using the MCNP software and a NaI(Tl) detector, at multiple source–detector distances and counting times. To assess stability and generalization, evaluation is performed on test sets created under conditions that differ from those of the training spectra including calibration variations without exposing the models to these conditions during training. In the first approach, the autoencoder compresses the 1,024-channel spectrum into a 16-dimensional latent space, which is then used as input for classification; however, in the second approach, the 1D-CNN utilizes all 1,024 channels for feature learning and decision-making. To analyze model behavior, interpretable methods such as feature importance analysis (SHAP) and visualization techniques t-SNE are employed. The results indicate that the autoencoder's latent representation provides more stable evidence across varying conditions than a 1D-CNN.

10.101: Mf-Toolkit: A Python Library for Efficient Multifractal Analysis

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Multifractal Detrended Fluctuation Analysis (MFDFA) is a vital tool for revealing hidden scaling complexity in non-linear time series. However, its high computational cost remains a major barrier for large-scale applications. We introduce mf-toolkit, an open-source library that solves this issue by using CPU-based parallelization and Numba acceleration to achieve highly efficient MFDFA. To demonstrate its robustness and performance, we apply MF-toolkit to analyze the complex, non-stationary acoustic patterns found in Humpback Whale vocalizations, showcasing its utility for accelerating physics research and advanced signal characterization.

11.101: Prediction of Pd, Pt, and Rh adsorption energies on graphene quantum dots using graph neural networks

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Transition metals such as Pd, Pt, and Rh exhibit excellent electrocatalytic activity but suffer from the disadvantages of being expensive and scarce. An effective strategy to optimize their use is to employ them as adatoms on suitable supports. In this context, graphene quantum dots (GQDs) are notable due to their abundance, large surface area, the presence of active edge sites, and interesting geometric structures, making them promising supports for electrocatalyst design. The interaction between these carbon-based systems and transition metals has shown promising results in improving stability and catalytic activity [1]. At the same time, artificial intelligence (AI) and machine learning (ML) are transforming materials design by enabling the efficient exploration of vast chemical and structural spaces, with computation times significantly shorter than conventional methods [2]. Within this context, graph neural networks (GNNs) have emerged as particularly suitable tools for modeling non-periodic atomic systems, as they explicitly capture connectivity, local interactions, and spatial symmetries without relying on periodic cells. Their application in materials science allows property prediction at substantially lower computational cost compared to conventional approaches [3]. In this work, density functional theory (DFT) calculations are combined with GNNs to predict the adsorption energies of Pd, Pt, and Rh on GQDs of different geometries. A database of adsorption configurations was generated, incorporating electronic, geometric, and charge properties. Each system was represented as a graph,with nodes corresponding to atoms and edges reflecting connectivity within a cutoff radius. As input attributes, we incorporate the previously calculated properties together with relative coordinates, atom type, and local chemical environment, which allows a more accurate representation of the relationship between structure and properties. Based on these representations, GNN models were trained and evaluated using specialized graph deep learning libraries. These networks update node states through a message-passing scheme in which each atom aggregates and transmits information from its neighbors to capture local environmental effects. For training, we employed MSE loss functions, global pooling strategies to obtain system-level descriptors, and graph convolution–based architectures, complemented by cross-validation to assess generalization. Preliminary results demonstrate good fitting and strong predictive performance, highlighting the potential of GNNs to accelerate property prediction and guide the rational design of new electrocatalysts. [1] Peng Y., Lu B., Chen S., ADV MATER, 2018, 30, 48, 1801995. [2] Mai H., Le T., Chen D., Winkler D., Caruso R., CHEM REV, 2022, 122, 16, 13478-13515. [3] Reiser P., Neubert M., Eberhard A., Torresi L., Zhou C., Shao C., Metni H., Van Hoesel C., Schopmans H., Sommer T., Friederich P., COMMUN MATER, 2022, 3, 93.

11.102: Data-Driven Identification of High-Performance Thermoelectric Materials Using Supervised Learning

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Machine learning (ML) is used to accelerate the discovery of novel functional materials by learning structure–property relationships from large datasets. This poster presents an ML-based approach for predicting and screening thermoelectric materials, with emphasis on systems containing lighter nuclei and low-dimensional compounds. Both regression models (to predict quantitative transport properties such as Seebeck coefficient and conductivity) and classification models (to distinguish high-performance from low-performance candidates) are employed. Feature engineering is performed using Matminer and ASE (Magpie, ElementProperty, Stoichiometry) and DScribe[1] descriptors(structural-property), with several training datasets drawn from density functional theory (DFT) calculations and open repositories. Early results indicate that regression models successfully reproduce trends in transport properties, while classification enables rapid identification of promising candidate materials. Future directions include incorporating phonon-derived features and exploring generative models to guide the design of new compounds. This framework illustrates the synergy between ab initio methods and ML for efficient thermoelectric materials discovery.

11.103: Data-Driven Estimation of ^{225}Ac Yield versus Irradiation Time and Current at Multiple Proton Energies

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Actinium-225 (^{225}Ac), a promising alpha-emitting radionuclide for targeted alpha therapy (TAT), offers a suitable half-life (9.9 days) and favorable decay chain, yet its limited availability hinders widespread clinical use. Proton irradiation of thorium-232 (^{232}Th(p,x)^{225}Ac) is a practical and efficient production method. This study utilized the TALYS-2.0 nuclear reaction model to simulate the excitation functions of the ^{232}Th(p,x)^{225}Ac reaction, with parameters optimized for better alignment with experimental cross section data. Additionally, two data driven models (Artificial Neural Network (ANN) and Support Vector Regression (SVR)) were developed to predict reaction cross sections using experimental datasets. The physical yield of ^{225}Ac was calculated via the integral yield formula at proton energies of 70, 90, and 150 MeV, evaluating yield as a function of irradiation time (at 250 μA beam current) and beam current (at 24 h irradiation). Results demonstrate that ANN and SVR models outperform TALYS, providing higher and more accurate yield predictions. These data driven approaches enhance the optimization of production parameters, paving the way for efficient ^{225}Ac generation to support clinical applications.

11.104: Deep Learning-Based Potential for Energy Prediction of SiC–H 2D Systems from Ab Initio Data

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The demand for greenhouse gas–free energy sources and high–efficiency catalytic materials has driven research into hydrogen storage and conversion. In this context, two–dimensional (2D) materials such as silicon–carbon (SiC) have emerged as promising candidates for hydrogen fuel cell applications due to their large surface area and tunable electronic properties. This study proposes a hybrid workflow combining ab initio calculations using the SIESTA package with deep learning techniques to construct a Machine Learning Potential (MLP) for the SiC–H system. A dataset of approximately 50,000 configurations generated from multiple DFT simulations—including atomic coordinates, forces, and energies—was reformatted for training a Deep Potential model. The trained model was subsequently integrated into LAMMPS and MC–MD simulations to investigate hydrogen adsorption energetics across various configurations. The deep learning model achieved a mean absolute error (MAE) of only a few meV per atom compared to DFT while offering orders of magnitude faster computation, significantly reducing simulation time. These results enable large–scale statistical simulations and provide a solid theoretical foundation for experimental studies on hydrogen storage and conversion.

11.105: Learning the Intrinsic Dimensionality of Fermi-Pasta-Ulam-Tsingou Trajectories using a Deep Autoencoder Model

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Recent studies have shown that the trajectories of the Fermi–Pasta–Ulam–Tsingou (FPUT) β model with $N = 32$ harmonic oscillators lie on a 2- or 3-dimensional Riemannian manifold for weak nonlinearities ($\beta \lesssim 1.1$). This conclusion was drawn using principal component analysis (PCA) applied to trajectory data comprising 4,000,000 data points. However, since PCA is inherently linear, it cannot capture nonlinear manifold structures. Here, we present a preliminary analysis of the same data using a deep autoencoder (DAE) with five hidden layers. The DAE outperforms PCA in reconstructing the trajectories and supports the earlier PCA-based findings.