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

Nguyen Van Hoa[1,*], Phan Thi Huong[1,2], Nguyen Tien Dung[1,2], Hoang Hai[3,4], Tran Thi Thu Hanh[1,2]

[1]*Laboratory of Computational Physics, Faculty of Applied Science, Ho Chi Minh City University of Technology (HCMUT), Ho Chi Minh City, 268 Ly Thuong Kiet Street, Dien Hong Ward, Ho Chi Minh City, Vietnam.*

[2]*Vietnam National University Ho Chi Minh City, Quarter 33, Linh Xuan Ward, Ho Chi Minh City, Vietnam .*

[3]*Institute of Fundamental and Applied Sciences, Duy Tan University, Tran Nhat Duat Street, District 1, Ho Chi Minh City, Vietnam.*

[4]*Faculty of Environmental and Natural Sciences, Duy Tan University, 03 Quang Trung Street, Da Nang, Vietnam.* **Email: nvhoa.sdh2412@hcmut.edu.vn*

INTRODUCTION

- Face-centered cubic (FCC) platinum crystal exhibits superior catalytic performance, particularly with its (100) surface facet. [1].
- Stable adsorption sites for hydrogen on Pt(100) were determined at bridge (B) and top (T) sites [2].
- Pt(100) surface is highly symmetric, so the Pt(100)-H system can be treated as an Ising-like model.

➔ How to quickly calculate the energy of each configuration as accurately as possible?

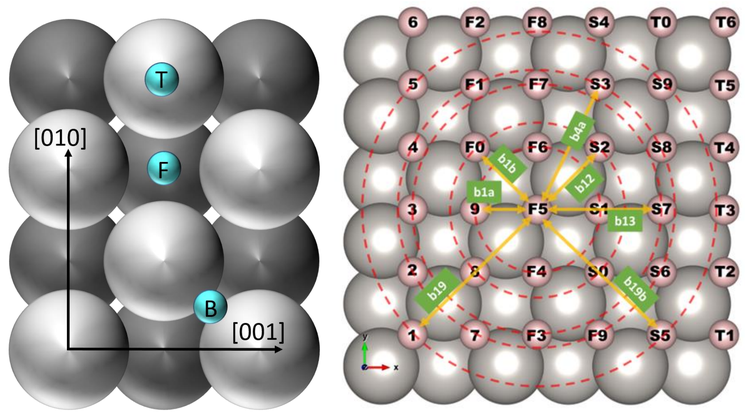

Figure 1. Hydrogen adsorption sites mapping on a symmetric Pt(100) surface [2].

[1] E. d. V. Gómez, S. Amaya-Roncancio, L. B. Avalle, D. H. Linares and M. C. Gimenez, Appl. Surf. Sci., 2017, 420, 1–8.

[2] V. H. Nguyen, M. P. Nguyen, T. V. Lam and T. T. H. Tran, Phys. Scr., 2022, 97, 035701.

METHOD

1) DFT data generation

$$E_{ads}(N_H) = E_{tot}(N_H) - E_{tot}(0) - \frac{N_H}{2}E_{H_2} = N_H \times E_{ads}(1) + E_{int}$$

- $E_{tot}(N_H)$ is the total energy of the SiC surface model adsorbing N_H hydrogen atoms.
- $E_{tot}(0)$ is the energy of the system without any adsorbed hydrogen atoms.
- E_{H_2} is the energy of a hydrogen molecule.
- E_{int} represents the interaction energy.

Density functional theory

siesta

- Exchange–correlation functional: GGA–PBE.
- Basis set: DZP.
- *k*-point grids: (3×3×1) MP.
- Maximum force tolerance: 0.02 eV/Å.
- Maximum displacement step: 0.02 Å.
- **80 hydrogen adsorption configurations considered.**

2) Regression

➢ **Multiple linear regression (MLR):**

$$E_{int} = \sum_i k_i \varepsilon_i \ \ with\ I_w = \begin{cases} 1 & if\ Ltot \geq threshold \\ 0 & if\ Ltot < threshold \end{cases}$$

➢ **Decision tree**: XGBoost.

➢ **Cluster expansion (CE) model** with LASSO algorithm.

$$E_{int} = J_0 + \sum_i J_i \Phi_i(\sigma) + \sum_{i<j} J_{ij}\Phi_{ij}(\sigma) + \sum_{i<j<k} J_{ijk}\Phi_{ijk}(\sigma) + \cdots$$

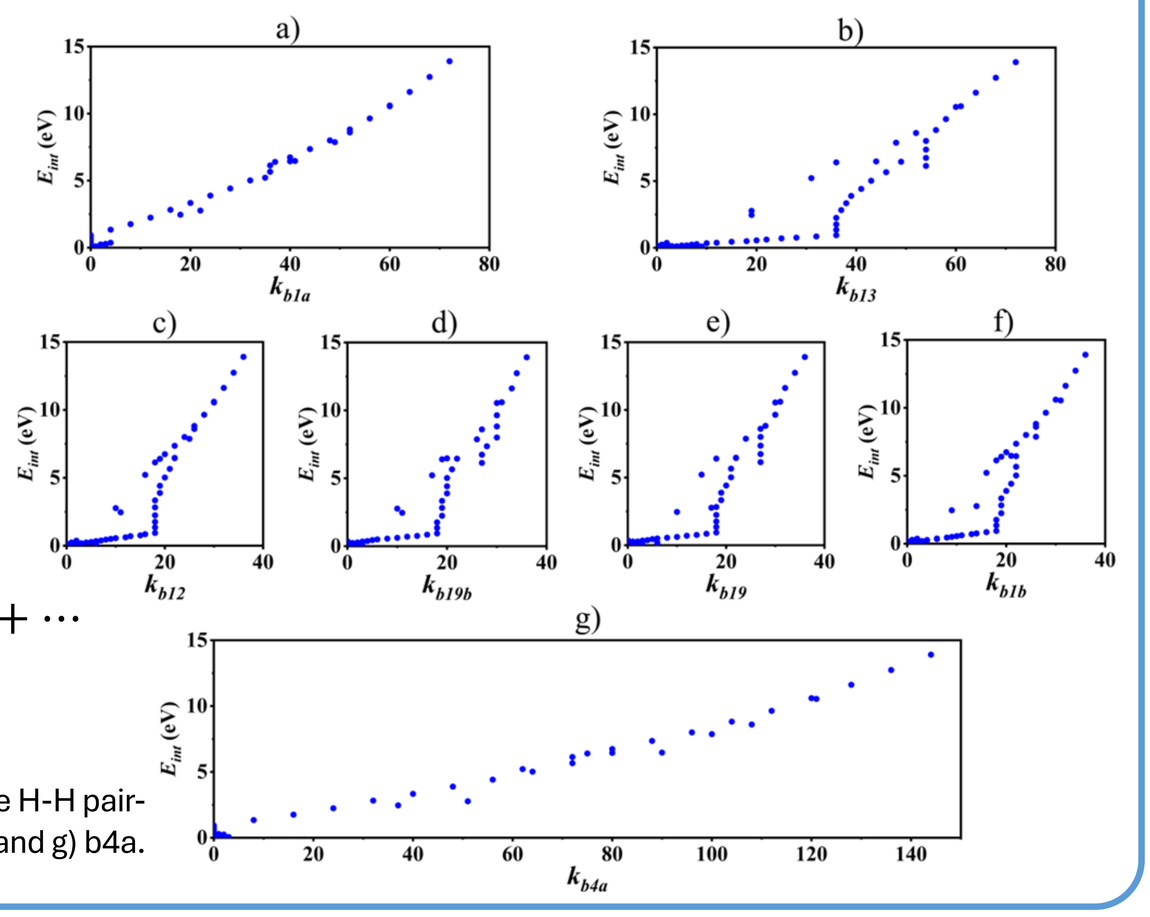

Figure 2. The scatter plots of the interaction energies from DFT data via the H-H pair-type number of: a) b1a, b) b13, c) b12, d) b19b, e) b19, f) b1b and g) b4a.

RESULTS

➢ **The interaction energy can be described as a simple function of regard hydrogen configuration.**

➢ **Multiple linear regression (MLR) M2 has the most accurate prediction.**

➢ **M2 and CE can capture the sudden increment in E_{int} of Pt(100)-H when H:Pt exceeds a 1:1 ratio.**

Table 1. The comparison between linear regression models (M0, M1, M2), XGboost, cluster expansion prediction.

Model	Adjusted R^2	AIC	Mean absolute error	Standard deviation of the absolute errors
MLR M0	0.994	65.53	0.2429	0.3169
MLR M1	0.999	-75.00	0.1601	0.3231
MLR M2	**0.999**	**-72.86**	**0.1329**	**0.1738**
XGBoost	-	-	0.1804	0.3359
CE	0.983	-	-	-