

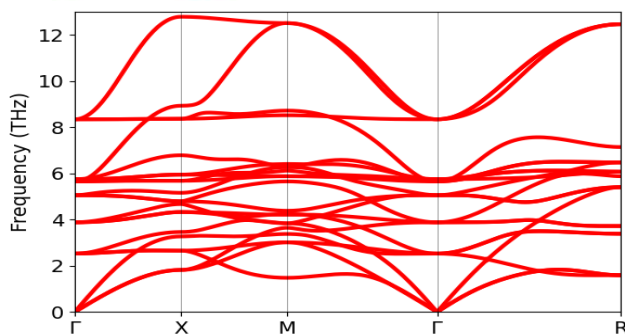
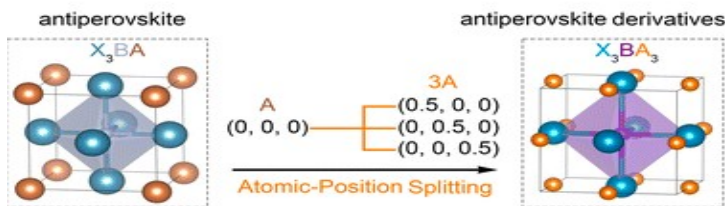


GW/BSE investigation of the electronic and optical properties of strained and unstrained Sr_3NF_3

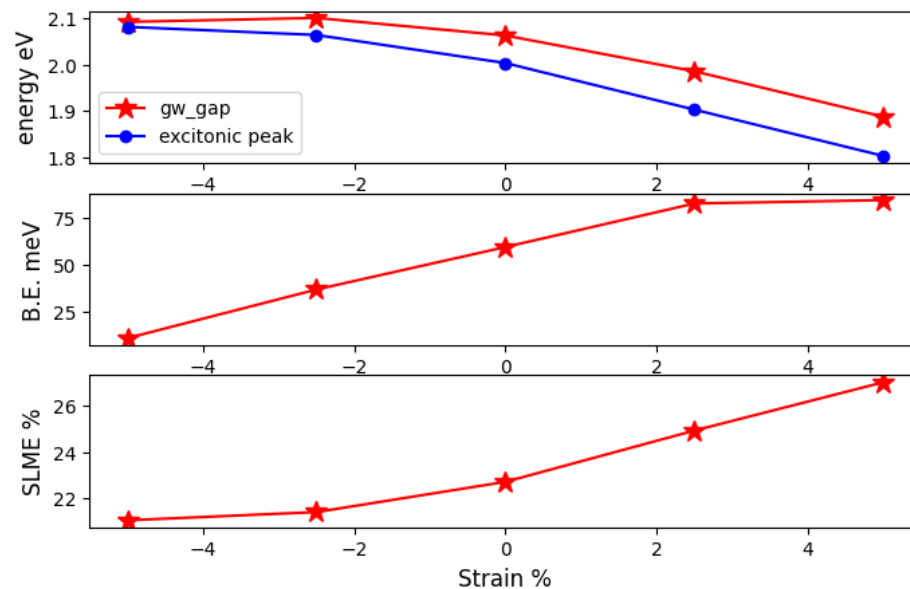
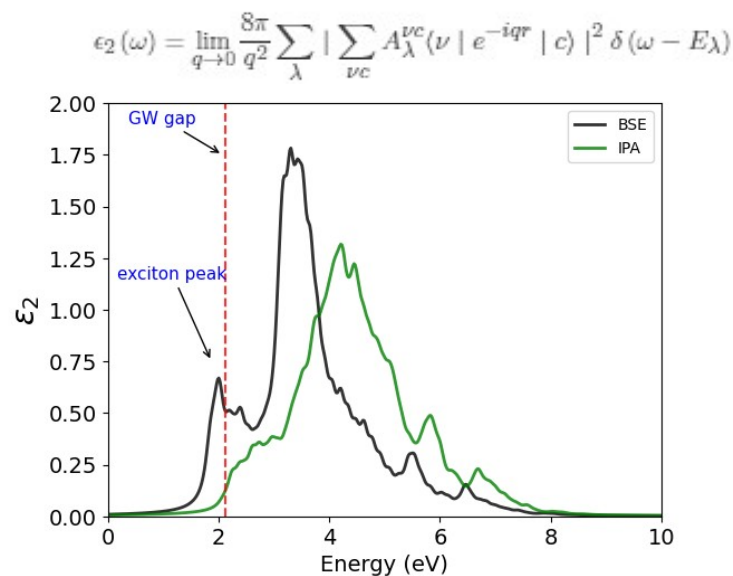
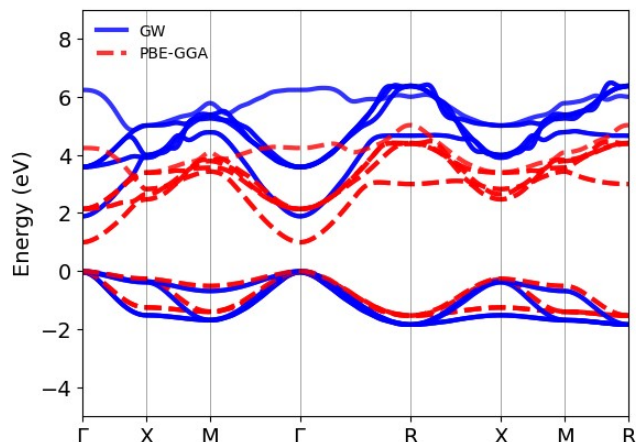
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Sr_3NF_3 is new variant of the antiperovskites with Pm3m symmetry.



$$E_{nk}^{qp} = \epsilon_{nk} + \langle \psi_{nk} | \Sigma(E_{nk}^{qp}) - V_{xc} | \psi_{nk} \rangle$$



PBE (GGA) gap (eV)	GW gap (eV)	Optical gap (eV)	Excitonic binding energy (meV)	Electron effective mass (mo)	Hole Effective Mass (mo)
1.16	2.06	2.00	59.2	0.41	0.55

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References:

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