Soutenance de thèse

Mardi 30 septembre 2025
14h00 – Amphithéâtre

Machine Learning-Driven First-Principles Modeling of Far-Infrared Materials

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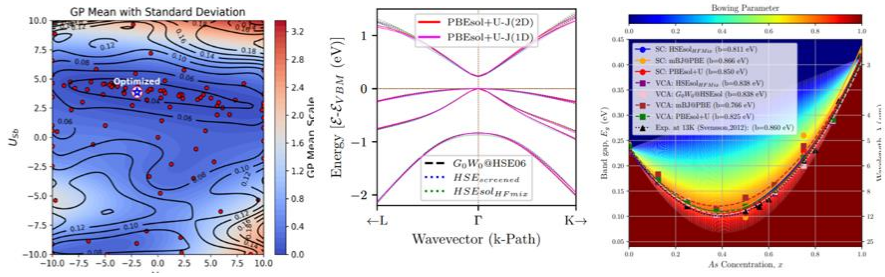
Abstract

This thesis focuses on the modeling of narrow-gap far-infrared semiconductors, ternary alloys, and heterovalent heterostructures. To overcome the limitations of conventional Density Functional Theory (DFT), a Bayesian Machine (BMach) framework [2] is developed to optimize internal DFT meta-parameters, such as the Hubbard U in DFT+U and the mixing (α) and screening (μ) parameters in hybrid exchange–correlation functionals. These parameters are benchmarked against quasiparticle corrections obtained from Green's function–based quasiparticle-GW (G_0W_0) calculations, with BMach employing Gaussian process regression (GPR) and physics-informed loss functions.

Applied to the benchmark semiconductors InSb and InAs, BMach accurately reproduces experimental band gaps, effective masses, and Luttinger parameters at significantly reduced computational cost [1]. The study further explores CuPt-ordered $InAs_xSb_{1-x}$ alloys across the full composition range using both supercell and Virtual Crystal Approximation (VCA) approaches; notably, the VCA-based G_0W_0 method yields a bowing parameter of 0.838 eV, in excellent agreement with experiment. Finally, the band alignment at the CdTe/InSb(001) heterointerface is determined using the potential-lineup method with BMach-calibrated parameters, confirming a type-I alignment consistent with experimental observations.

This work establishes a transferable and extensible computational framework for high-fidelity electronic-structure predictions across diverse material systems, with direct relevance for future electronic, optoelectronic, energy, and quantum technologies.



1. **Ritwik Das**, AS G.-J., and F.Aniel, "High-fidelity electronic structure and properties of InSb: G_0W_0 and Bayesian-optimized hybrid functionals and DFT+U approaches", *Physical Review B, 112, 075136* (American Physical Society) (2025).
2. **Ritwik Das**, "BMach: a Bayesian machine for optimizing Hubbard U parameters in DFT+U with machine learning", *arXiv, arXiv:2407.20848* (**2024**).