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Alpesh Sheth

PhD · Computational Condensed Matter Physics

Computational physicist working on the electronic structure of quantum materials. I construct effective multi-orbital models for correlated-electron systems, compute them with many-body and first-principles methods on high-performance computing infrastructure, and transfer the same modeling discipline to applied problems in machine learning and optimization.

EXPERIENCE

Doctoral Researcher Dec 2021–Nov 2025
Laboratoire Ondes et Matière d'Aquitaine (UMR 5798, CNRS), Université de Bordeaux

- Constructed effective multi-orbital models separating the electronic physics of infinite-layer nickelates ($RNiO_2$) from high-T_c cuprates.
- Identified robust antiferromagnetic and charge-order tendencies driven by Fermi-surface nesting.
- Developed and optimized Python and Fortran modules for quantum-material simulation; workflow automation on high-performance computing clusters reduced compute time by approximately 35 %.
- Designed scalable frameworks to validate theoretical predictions against experimental data for complex material properties.

Research Intern, Data Science Jun 2022–Nov 2022
Uresearcher

- Automated data-extraction pipelines through public interfaces, reducing manual pre-processing by approximately 70 %.
- Applied predictive machine-learning models to drug-design datasets, improving hit-prediction accuracy by approximately 15 %.
- Mined open-source molecular databases to identify candidate molecules for targeted applications.

Research Fellow Apr 2020–Nov 2021
The Maharaja Sayajirao University of Baroda

- Performed density functional theory and molecular dynamics simulations of boron-based nanomaterials for radiation shielding.
- Designed modular high-performance computing workflows across more than twenty structural parameter sets, accelerating design cycles by approximately 50 %.
- Presented a density-functional study of twisted graphene and hexagonal boron nitride moiré heterostructures at ICAFMOD 2020.

Research Intern Jun 2018–Nov 2021
Physical Research Laboratory

- Computed the non-linear alternating-current admittance of materials, improving predictive reliability by approximately 40 % over prior approaches.
- Analyzed transport properties through the density of states using second-order perturbation theory and the Kubo formalism.
- Determined critical size thresholds for superconducting nanoparticles used in magnetic sensor design.

EDUCATION

PhD in Material Science 2021–2025
Université de Bordeaux

MSc in Condensed Matter Physics 2018–2020
The Maharaja Sayajirao University of Baroda

BSc in Physics 2015–2018
The Maharaja Sayajirao University of Baroda

PUBLICATIONS

- **A. Sheth** et al., *Emergence and tunability of Fermi-pocket and electronic instabilities in layered Nickelates*, Journal of Physics: Condensed Matter **37**, 125703 (2025). doi:10.1088/1361-648X/ada908
- **A. Sheth**, *Theoretical modelling of infinite-layer nickelates*, PhD thesis, Université de Bordeaux (2025). theses.hal.science/tel-05502836
- B. Devanarayanan, A. Sharma, **A. Sheth** et al., *Background for the Self Consistent Renormalisation (SCR) Theory*, arXiv:2108.12683 (2021).

INVITED TALKS

- *Modelling oxygen and rare-earth atomic impurities in nickelates*, IIP-Natal WE-Heraeus Workshop on New Frontiers in Emergent Materials (2023). Recording available.

SELECTED PROJECTS

- **Quantum Portfolio.** Full-stack application for portfolio optimization mapped onto the Ising model: live market data ingestion, constraint penalties for sector exposure and cardinality, a tunable risk-aversion parameter, and simulated annealing with variational free-energy tracking.
- **Graphene heterostructures.** Electronic properties of twisted graphene and hexagonal boron nitride bilayers from density functional theory, including moiré superlattice effects.

TECHNICAL SKILLS

Languages	Python, C++, Fortran, Julia, Bash, MATLAB, LaTeX
Many-body methods	Green's functions, dynamical mean-field theory, exact diagonalization, second-order perturbation theory, Kubo formalism
Simulation packages	VASP, Quantum ESPRESSO, LAMMPS, CP2K, TRIQS
Data and machine learning	predictive modeling, statistical analysis, automated data pipelines
Infrastructure	high-performance computing (Slurm), Git, workflow automation