Ritwik Das, PhD | Curriculum vitae

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C2N, French National Centre for Scientific Research (CNRS) – Université Paris-Saclay

Google Scholar (ID: H2ZhTsEAAAAJ) | **ResearchGate** (ID: Ritwik-Das-3)

• Materials Science • Computation, Sumulation, Experiment • Condensed Matter • Semiconductor Devices • First-Principles Modeling • AI/ML • Optimization • TCAD/EDA • Automation • Teaching, Mentoring

Physicist and materials scientist with a strong foundation spanning **theory, simulation, and computational physics** to **experiments, characterization, and semiconductor device engineering**. Experienced in bridging **cleanroom-based fabrication and electrical measurements** with **first-principles simulations** and **machine-learning–driven optimization frameworks**. Developed and applied **Bayesian, machine-learning, and deep-learning approaches** for parameter calibration in **DFT+U** and **hybrid-functional calculations**, achieving high-fidelity predictions across **III–V and II–VI semiconductors**. Skilled in **sensor and MEMS design**, **device characterization**, and **IC layout and verification** using **Cadence, Silvaco, and COMSOL**. Passionate about combining **physics-based understanding** with **data-driven methods** to accelerate **materials discovery and device innovation**.

EDUCATION QUALIFICATIONS

- **Doctor of Philosophy (PhD) in Theoretical & Computational Physics, Materials Science** **2025**
  Université Paris-Saclay — C2N — CNRS *Paris, FRANCE*
  Thesis on: *Machine Learning-Driven First-Principles Modeling of Far-Infrared Materials*
- **Master of Science (M.Sc.) in Nanophysics** **2021**
  École Polytechnique, Université Paris-Saclay *Paris, FRANCE*
  In collaboration with: École Normale Supérieure (ENS) Paris-Saclay, CentraleSupélec, & Institut d'Optique
- **M.Sc. in Electrical & Electronic Engineering (EEE)** **2018**
  École Polytechnique Fédérale de Lausanne (EPFL) *Lausanne, SWITZERLAND*
  Specialization: Microelectronics and Nanotechnology
- **Electronics Engineering** **2017**
  Nanyang Technological University (NTU) *SINGAPORE*
  Specialization: Integrated Circuit Design. *Exchange at Technical University of Munich (TUM)* *GERMANY*

PROGRAMMING LANGUAGES

- Python
- Matlab
- C/C++
- Embedded C
- LaTeX
- Julia (*newbie*)
- HTML
- Java
- VHDL
- Verilog

SOFTWARE & TOOLS

- **Quantum Chemistry Methods:** *HF, DFT (LDA, GGA, meta-GGA, hybrid), mBJ, GW, DFT+U, pseudopotential generation (Ultrasoft, PAW, ONCV), perturbation theory (DFPT), Electron-Phonon, Dataset Generation for AI-ML/post-DFT processing*
- **Ab Initio Computational Tools:** *Quantum Espresso (QE), VASP, BerkeleyGW, EPW, Wannier90, BoltzTraP2, Yambo*
- **HPC:** *MPI, SLURM, cluster job scripting*
- **DevOps, Version Control & Automation:** *Python (Collaborative), Git, GitHub/GitLab, Docker, CI/CD pipelines*
- **Operating Systems:** *Linux, Windows, macOS*
- **Layout, Design & Simulation Tools:** *KLayout, Silvaco, ANSYS, COMSOL, SCAPS*
- **Machine Learning & Scientific Computing:** *Python, NumPy, Pandas, SciPy, Scikit-learn, Matplotlib, Seaborn, Scikit-optimize, Optuna*
- **Deep Learning for Science & AI Integration:** *PyTorch, Graph Neural Networks (GNNs)*
- **Optimization & Statistical Modeling:** *Gaussian Processes, Bayesian Methods, Surrogate Modeling, Kernel methods, Acquisition function, UQ, CMA-ES, Differential Evolution (DE)*
- **Productivity, Writing & Graphics:** *LaTeX, VSCode, Inkscape, Microsoft Office*

RESEARCH EXPERIENCE & PROJECTS

1. Materials-Modeling Projects

- **Strain-Coupled Electronic Structure and Deformation Potential Analysis**

C2N-CNRS, Paris-Saclay **2024–2025**

- Performed systematic hydrostatic, uniaxial, and biaxial strain calculations for InSb by applying well-defined lattice deformations in DFT, with internal atomic relaxations where appropriate.
- Tracked strain-induced shifts and splittings of Γ-point band edges and extracted deformation potentials from the linear strain–energy response.
- Quantified the coupling between mechanical strain and band-gap modification, establishing a consistent strain–band-structure mapping relevant for continuum-level or device-level modeling.

- **Band Alignment at the CdTe/InSb Heterointerface using First-Principles (DFT)**

C2N-CNRS, Paris-Saclay **2022–2024**

- Modeled **CdTe(001)**, **InSb(001)**, and their heterostructure using mBJ, DFT+U, and hybrid functionals.
- Applied the **potential-lineup method** to determine **valence and conduction-band offsets** and analyzed **interface dipole formation**.

- **First-Principles Studies of Bulk and Alloyed III–V / II–VI Semiconductors**

C2N-CNRS, Paris-Saclay **2020–2023**

- Computed **band structures, DOS, and effective masses** using **PBEsol+U, HSEsol, mBJ, and G_0W_0**.
- Modeled **InAsSb alloys** via **ordered supercells** and **VCA**, incorporating spin–orbit coupling and band-unfolding analysis.

- **Pseudopotential Generation and Benchmarking**

C2N-CNRS, Paris-Saclay **2019–2022**

- Generated and validated **ONCV, PAW, and ultrasoft pseudopotentials** including semicore 4d states.
- Benchmarked results against **all-electron references** to ensure accuracy and transferability.

- **Topological Materials and Quantum Anomalous Hall Systems**

C2N-CNRS, Paris-Saclay **2019–2021**

- Chern numbers, Berry curvature, and magnetic parameters via DFT+U and Python postprocessing.
- Modeled quantum phase transitions and spin–orbit effects in data-rich material systems.

- **Monte Carlo Simulation of Fermi–Dirac Distributions in 2D**

École Centrale Paris (CentraleSupélec), France **2019–2020**

- Simulated **temperature-dependent carrier statistics** in 2D electron systems using **Monte Carlo methods** for transport analysis.

2. AI, Machine Learning, and Optimization for Materials Modeling

- **Deep-Learning Pipeline for *Ab Initio* Parameter Inference**

C2N-CNRS, Paris-Saclay ***2025***

- Developed a **deep-learning pipeline** (MLP → GNN) to infer **Hubbard U** and related simulation parameters from atomic and electronic descriptors.
- Automated **data ingestion, training, and validation** using Python and HPC workflows for near-real-time prediction within **DFT+U** simulations.
- Extended the **BMach Bayesian framework** toward scalable, AI-assisted *ab initio* modeling.

- **Machine Learning-Driven U Prediction from Ab Initio Datasets**

C2N-CNRS, Paris-Saclay ***2024 - 2025***

- Developed a **deep-learning pipeline** (MLP → GNN) to infer **Hubbard U** and related simulation parameters from atomic and electronic descriptors.
- Automated **data ingestion, training, and validation** using Python and HPC workflows for near-real-time prediction within **DFT+U** simulations.
- Extended the **BMach Bayesian framework** toward scalable, AI-assisted *ab initio* modeling.

- **Bayesian Optimization Framework for *Ab Initio* Parameter Calibration (BMach)**

C2N-CNRS, Paris-Saclay **2022–2024**

- Created **BMach**, a **Gaussian-process Bayesian optimization** system for automated **Hubbard U** tuning in **DFT+U**.
- Integrated **uncertainty quantification** and **acquisition-function strategies (EI/UCB)** to enhance exploration–exploitation balance.
- Validated accuracy across **bulk and alloy semiconductors**, benchmarked against **G_0W_0** results.

3. Device-Level Projects

- **TLM Design and Electrical Parameter Modeling**

Centre for Nanosciences and Nanotechnologies (C2N-CNRS), Paris-Saclay **2020–2024**

- Designed **circular (CTLM) and linear TLM structures** in **Silvaco Atlas** and **KLayout** to analyze metal–semiconductor contacts.
- Performed **I–V characterization** and **low-temperature cryogenic measurements** to study carrier transport and contact resistance.
- Built a **Python-based analytical model** (Bessel-function formalism) to extract **contact resistance, transfer length, and sheet resistance**, calibrated against experimental data.
- Compared experimental and simulated results to optimize **metal–semiconductor interface behavior**.

- **Sensor Fabrication and Characterization: Pressure and Water-Quality Monitoring Devices**

EPFL (Lausanne, Switzerland), CIME Nanotech – MINATEC (Grenoble, France) **2017–2019**

- Fabricated **piezoresistive MEMS pressure sensors** on Si and SOI wafers using oxidation, lithography, RIE, ion implantation, and annealing in a cleanroom environment.
- Performed **profilometry, ellipsometry, and four-probe resistivity** measurements for dopant and layer characterization.
- Conducted a **feasibility study of polymer-based OFET arrays** with **PANI, PEDOT, and PPy** layers on flexible substrates for multi-ion detection.
- Designed **multiplexed readout electronics** and packaging for in-situ, low-cost water-quality assessment.

- **MEMS Micropump for Drug Delivery**

EPFL (Switzerland), Politecnico di Torin (Italy) **2017**

- Designed a **silicon-based MEMS micropump** for precision drug delivery.
- Simulated **fluid dynamics and magnetic actuation** in **COMSOL Multiphysics**, defining microchannel geometry and diaphragm motion.

4. Electronics and Integrated-Circuit Design

- **Advanced CMOS Integrated-Circuit Design Projects**

Nanyang Technological University (NTU), Singapore **2015–2017**

- **FSM Design (AMS 0.35 µm CMOS):** Built a Verilog control circuit, performed RTL synthesis, and analyzed power/timing.
- **Matrix Multiplier and Adder Logic:** Implemented RTL architectures; completed DRC/LVS checks and timing closure.
- **Pseudo-Random Sequence Generator:** Designed 4-bit and 6-bit LFSRs; verified functionality using **Synopsys** tools and physical verification.
- **Differential Wideband Amplifier:** Designed a fully differential analog amplifier; ran post-layout parasitic simulations for high-frequency operation.
- **7 nm FinFET Full Adder:** Implemented at the 7 nm node using **Cadence Encounter**; executed place-and-route, STA, and power profiling.

5. Telecommunication

- **CDMA Wireless Mobile Optical Communication System**

Jadavpur University, Kolkata, India **2013–2015**

- Developed an **IR-based low-speed wireless communication system** using **CDMA encoding** with **Maximum-Length Sequence (MLS)** and **Gold Codes** for multiplexed transmission.

PROFESSIONAL/WORK EXPERIENCE

- **Scientific Consultant (Reviewer)** ***2025***
  Remote *California, USA*
- **Teaching Fellow (Adjunct University Instructor)** ***2021 –2024***
  École Polytechnique, Université Paris-Saclay *Orsay, FRANCE*
- **Visiting Researcher** ***2018***
  University of Calcutta *Kolkata, INDIA*
- **Research Engineer** ***2018***
  EPFL, CIME Nanotech *Lausanne (Switzerland), Grenoble (France)*
- **Research Associate** ***2015 – 2017***
  Nanyang Technological University (NTU) *Singapore*

- **Summer Intern** — ***2013***
  Airports Authority of India (AAI), NSCBI Airport — *Kolkata, INDIA*
- **Winter Intern** — ***2012 – 2013***
  Prasar Bharati (Broadcasting Corporation of India): All India Radio (AIR) — *Kolkata, INDIA*
- **Robotics Intern** — ***2012***
  Robosapiens India Pvt. Limited — *Kolkata, INDIA*

ONLINE RESEARCH PROFILES & PUBLICATIONS

- **Google Scholar**– User ID: H2ZhTsEAAAAJ
- **ResearchGate** – User ID: Ritwik-Das-3

The following also includes articles currently under peer review or in preparation:

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**, AS G.-J., and F.A., **"Structural, Electronic Properties and Band Gap Bowing Parameters of CuPt-Ordered $InAs_xSb_{1-x}$ Alloys: First-Principles Insights from HSE, G_0W_0, mBJ, and DFT+U"**. Submitted to *Physical Review Materials* (APS) (**2025**).
3. **Ritwik Das**, AS G.-J., and F.A., **"First-principle calculations of the band alignment at the CdTe/InSb (001) heterointerface"**. *In preparation*; to be submitted. (**2025**).
4. **Ritwik Das**, **"BMach: a Bayesian machine for optimizing Hubbard U parameters in DFT+U with machine learning"**, *arXiv preprint, arXiv:2407.20848* (**2024**).
5. **Ritwik Das**, A. S., and I. D., **"Topological Phase Transitions in Kagome Ferromagnets: The Role of Intrinsic Rashba Spin-Orbit Coupling"**, *arXiv preprint, arXiv:2502.06686* (**2025**).
6. **Ritwik Das**, S.B., and I.D., **"In-plane magnetization orientation driven topological phase transition in $OsCl_3$ monolayer"**, *Electronic Structure, 6(2), 025005* (IOP) (**2024**).
7. **Ritwik Das**, A.-S. G.-J., and F. Aniel, **"Bayesian Machine: Optimizing the Hubbard U Parameter in DFT+U With Machine Learning"**, *European Materials Research Society (E-MRS) Conference*, **2023**.
8. S.B., F.L.B., **Ritwik Das**, F.G.U., N.T., et al., **"Exchange interactions and spin dynamics in the layered honeycomb ferromagnet"**, *Physical Review B, 105(18), 184430* (APS) (**2022**).
9. V.S.S., **Ritwik Das**, and A.R., **"Numerical investigation of jet agitation in a nuclear liquid waste storage tank"**, *Progress in Nuclear Energy, 109, 204–213* **(2018)**.
10. **Ritwik Das** and A.S., **"Designing a Universal GNSS Simulator for Pseudorange Calculation"**, *International Journal on Recent and Innovation Trends in Computing and Communication, 3(1), 382–388* **(2015)**.

AWARDS AND ACHIEVEMENTS

- **Competitive National Doctoral Fellowship (MESRI, France):** *Awarded through national selection by the French Ministry of Higher Education and Research* ("Ministère de l'enseignement supérieur, de la recherche et de l'innovation"*), providing full funding and salary support for my PhD project on ML-driven DFT and quantum chemistry.*
- **Master's Scholarship:** *Awarded scholarship for the whole span of Master's studies in France.*
- **Charpak Scholarship:** *Awarded by the French Embassy in Delhi, India, covering my stay in France.*
- **Singapore Government Scholarship:** *Received a government scholarship from Singapore during my Master's at NTU.*
- **National Talent Recognition:** *Achieved national recognition in India's National Talent Search Examination (NTSE).s*
- **Technical Competition Success:** *Won 2nd prize at the KSHITIJ 2012, the largest technical fest in Asia, hosted by the Indian Institute of Technology (IIT), Kharagpur.*
- **Science:** *Placed 2nd in the National Science Talent Search at the state level in the state of West Bengal in India.*

LANGUAGES

- **English** ●●●●● *Native or bilingual proficiency*
- **Bengali** ●●●●● *Native or bilingual proficiency*
- **Hindi** ●●●●○ *Moderate working proficiency*
- **French** ●●○○○ *Elementary proficiency (A1/A2 level)*