HEMANT VERMA

Ph.D. Candidate, Computational Semiconductor Physics - Thin Film Materials, Metallization & Transport
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PROFESSIONAL SUMMARY

Materials scientist specializing in **metal thin films for semiconductor technology**: electronic structure, **resistivity and carrier scattering physics, electron-phonon coupling, and interface engineering** in metallization-relevant systems (**TiN, NbN**). Combines **first-principles modeling (DFT, Boltzmann transport, DFT+NEGF)** with hands-on **thin film processing experience (PVD thermal evaporation, spin coating, spray coating)** from solar cell device fabrication. Skilled in **root-cause analysis of process-property relationships**, HPC-driven simulation workflows, and Python automation - connecting material chemistry, film orientation, and interfaces to **electrical performance (resistivity, mobility, carrier lifetimes)** for advanced interconnect and device scaling.

CORE TECHNICAL COMPETENCIES

- **Metal thin films & metallization physics:** resistivity and mobility-limiting mechanisms, carrier scattering, orientation-dependent transport in TiN/NbN; physics directly applicable to interconnect metals (Cu, W, Mo, Ru alternatives)
- **Thin film deposition (hands-on):** PVD (thermal evaporation of metal electrodes), spin coating, spray coating for solar cell device fabrication; working knowledge of ALD/CVD process principles
- **Interfaces & contacts:** work function analysis, band alignment, metal-semiconductor contact study (DFT+NEGF), thin-film orientation dependence
- **Electron-phonon coupling:** EPC matrix elements, scattering rates, carrier lifetime extraction across temperature regimes
- **Electronic structure engineering:** band structure, DOS, effective mass trends, Fermi-level dependent behavior
- **Transport modeling:** Boltzmann transport formalism, anisotropic transport interpretation, mobility trends
- **Optical response:** dielectric function, absorption spectra, electronic transition analysis
- **Characterization data analysis & root-cause analysis:** linking material chemistry and process conditions to measured electrical/optical properties
- **HPC & automation:** parallel DFT workflows, convergence optimization, Python post-processing pipelines, Slurm/PBS

RESEARCH EXPERIENCE

Ph.D. Researcher - Metal Thin Films: Electronic Structure, EPC & Transport 2021-Present
Research Center for Applied Sciences (RCAS), Academia Sinica | National Taiwan University, Taiwan

- Performed large-scale DFT simulations (VASP, Quantum ESPRESSO, JDFTx) to characterize electronic structure and carrier behavior in TiN and NbN metal thin films, including thin-film and crystal-orientation-dependent trends relevant to low-resistivity metallization.
- Computed electron-phonon coupling (Wannier90 + EPW) to extract scattering rates and carrier lifetimes, enabling physics-based root-cause interpretation of mobility- and resistivity-limiting mechanisms in metal films.
- Modeled anisotropic carrier transport using Boltzmann transport formalism; linked crystallographic orientation to transport and relaxation pathways - key physics for interconnect line resistance at scaled dimensions.
- **Supervising a DFT+NEGF metal-semiconductor contact study** of CrS_2 (TMD) with SnSe monolayers for thermoelectric devices: contact resistance, interface electronic structure, and band alignment.
- Built automated Python post-processing pipelines for band/DOS analysis, EPC-derived lifetime statistics, and optical property visualization.
- Executed production-scale simulations on HPC clusters (Slurm/PBS); optimized convergence strategy (k-point sampling, smearing, cutoff, parallel efficiency) for reliable, reproducible trends.

Thin Film Processing & Device Fabrication - Solar Cells (hands-on)

- Fabricated thin-film solar cell devices: **PVD metallization via thermal evaporation of metal electrodes**, plus solution-based thin film deposition by **spin coating and spray coating**.
- Gained practical understanding of deposition process windows, film uniformity, and process-performance coupling in device stacks - complementing first-principles process interpretation.

M.Sc. Thesis - Strain-Induced Band Engineering in 2D Semiconductors 2019-2021
Department of Physics, IIT Jodhpur, India

- Modeled strain-dependent bandgap and band alignment tuning in Janus WSSe monolayers using DFT.
- Predicted photocatalytic activity changes by correlating electronic structure modulation with redox potential alignment.

EDUCATION

Ph.D. in Physics - National Taiwan University, Taiwan 2021-Present
Taiwan International Graduate Program (TIGP), Academia Sinica - Computational Materials Science | CGPA: 3.94/4.3

M.Sc. in Physics - Indian Institute of Technology (IIT) Jodhpur, India 2019-2021
CGPA: 8.14/10

SELECTED PROJECTS (DEVICE-RELEVANT FIRST-PRINCIPLES MODELING)

- **EPC-limited relaxation in TiN/NbN metal films:** quantified temperature-dependent scattering rates and carrier lifetimes; analyzed anisotropy vs. crystal orientation for thin-film transport and resistivity interpretation.
- **Metal-semiconductor contact engineering (supervision):** DFT+NEGF study of CrS_2/SnSe monolayer contacts for thermoelectric devices - interface transmission, contact behavior, and band alignment.
- **Optical response modeling:** computed dielectric function/absorption spectra and interpreted transition-driven spectral shifts in doped layered semiconductors.

TECHNICAL SKILLS

- **Methods:** DFT, GW, Wannier interpolation, electron-phonon coupling, Boltzmann transport, NEGF (quantum transport)
- **Thin film processing:** PVD (thermal evaporation), spin coating, spray coating; deposition process fundamentals (ALD/CVD/PVD)
- **Software:** VASP, Quantum ESPRESSO, JDFTx, EPW, Wannier90
- **Programming:** Python (NumPy, Pandas, Matplotlib), Bash, Git
- **HPC:** Slurm/PBS job scripting, parallel computing, convergence optimization
- **Visualization:** VESTA, XCrySDen

SELECTED RESEARCH IMPACT

- Quantified EPC-limited carrier lifetimes across temperature regimes for metallic thin films (TiN, NbN).
- Identified orientation-dependent anisotropic scattering pathways in TiN thin films - informing how film texture impacts resistivity.
- Demonstrated strain-induced bandgap modulation in 2D semiconductors for electronic property tuning.

PUBLICATIONS

1. P. Srivastva, B. Bazri, Y.-T. Hung, **H. Verma**, et al., Probing Interfacial Chemistry of Functionalized Ceramic Nanoparticles to Optimize Li^+ Pathways in Polymer Electrolytes for Solid-State Lithium Metal Batteries, **Nano Energy** 146 (2025) 111559.
2. L. T. Ngo, Y.-T. Huang, C.-C. Chang, **H. Verma**, et al., High-Efficiency and Ultrastable Solvent-Free Curable Perovskite Quantum Dot Inks for MicroLED and LED Backlighting Applications, **Nano Energy** 142 (2025) 111230.
3. L. T. Ngo, W.-T. Huang, **H. Verma**, et al., Hybrid-Protected Perovskite Quantum Dot Films with Ultra-High Efficiency and Stability for LED Backlighting, **ACS Applied Materials & Interfaces** 16(48): 66262-66272 (2024).
4. A. Thakran, A. Mohapatra, **H. Verma**, et al., Cascaded-Type Band Alignment of a WBG Perovskite/NBG Perovskite for Heterostructure Solar Cells, **ACS Applied Energy Materials** 7(8): 3039-3048 (2024).
5. **H. Verma**, A. J. Kale, et al., Enhanced Photocatalytic Activity in Strain Engineered Janus WSSe Monolayers, **Journal of Electronic Materials** 50, 7230-7239 (2021).

MANUSCRIPTS UNDER REVIEW / SUBMITTED

1. **H. Verma**, T.-Y. Peng, et al., *Anisotropic Hot Carrier Relaxation Mediated by Electron-Phonon Scattering in TiN Thin Films*, under review in **Surfaces and Interfaces** (2026).
2. **H. Verma**, S.-C. Huang, C.-C. Kaun, *Electronic and Optical Responses in BA_2PbBr_4: From Semiconductor to Half-Metal via 3d Transition-Metal Doping*, submitted to **Surfaces and Interfaces** (2026).

HONORS AND AWARDS

- Best Paper Award, Center for Theoretical Physics, NTU (2025)
- TIGP Fellowship, Academia Sinica (2021-Present)
- Rajiv Gandhi Academic Scholarship, Govt. of India (2023)
- INSPIRE Scholarship, Top 1% in HSC Board (2016)

CONFERENCES, SUMMER SCHOOLS AND WORKSHOPS

- **H. Verma**, T.-Y. Peng, Y.-H. Chan, Y.-J. Lu, C.-C. Kaun, *Orientation-Dependent Hot Carrier Relaxation in TiN Thin Films Facilitated by Electron-Phonon Scattering*, 26th Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-26), Tsukuba, Japan, Oct 2025. (Poster P-196)
- **H. Verma**, T.-Y. Peng, Y.-H. Chan, Y.-J. Lu, C.-C. Kaun, *Impact of Crystal Orientation on Hot Carrier Lifetimes in Titanium Nitride*, Taiwan Physical Society Annual Meeting, National Sun Yat-sen University, Kaohsiung, Taiwan, Jan 2025. (Poster; supported by Academia Sinica)
- Summer School on First Principles Computational Materials - Advanced Level, National Tsing Hua University, Hsinchu, Taiwan, 2024. (Supported by NCTS)
- 22nd Workshop on First-Principles Computational Materials Physics, Tainan, Taiwan, Aug 22-23, 2024. (Supported by NCTS)