Dr. Vinod Kumar Solet

Senior Assistant at IOP Zagreb, Croatia

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Research Profile

Computational condensed matter physicist specializing in first-principles electronic structure methods and many-body perturbation theory (MBPT). My research focuses on predicting electronic, optical, and transport properties of semiconducting materials for energy and optoelectronic applications. I have strong expertise in excitonic effects, electron–phonon interactions, phonon-phonon interactions, defect physics, magnetic properties and high-performance computing (HPC).

Research Experience

Senior Assistant Oct. 2026–now
Institute of Physics Zagreb, Croatia

- Working on the HrZZ project "Soft-phonon physics and electron-phonon fluctuations in layered two-dimensional systems ".

Institute Research Fellow July 2025– July 2026
Indian Institute of Technology (IIT) Mandi, India

Doctoral Researcher (Ph.D.) Aug 2021– Oct 2025
Indian Institute of Technology (IIT) Mandi, India

- Performed DFT, *GW*, and BSE calculations for semiconductors
- Investigated quasiparticle and excitonic effects
- Wrote Python code to obtain defect-limited solar cell efficiency
- Studied thermoelectric materials using electron–phonon and phonon-phonon interactions
- Used HPC workflows for large-scale first-principles simulations

Technical Skills

Electronic Structure Methods: DFT, DFPT, DFT+U, GW, Bethe–Salpeter Equation (BSE), Electron–Phonon Coupling, and phonon-phonon interaction

Software: ABINIT, Wien2k, Exciting, Quantum ESPRESSO, YAMBO, BerkeleyGW, EPW, Phonopy, Phono3py, BoltzTraP/BoltzTraP2

High-Throughput & Structure Prediction: AFLOW, USPEX

Programming: Python (proficient), FORTRAN (basic)

Computing: HPC, parallel simulations, workflow optimization

Education

Indian Institute of Technology (IIT) Mandi, India **Aug-2021 to Oct-2025 (4 year)**

Ph.D. in Computational Materials Science

Advisor: **Dr. Sudhir Kumar Pandey**

Thesis title: Understanding and Predicting Properties of Semiconductors for Photovoltaic and Thermoelectric Devices using *ab initio* Many-body Perturbation Theory

Indian Institute of Technology (IIT) Mandi, India **2019–2021**

M.Sc. in Physics

RRBMU Alwar, India **2015–2018**

B.Sc. in Physics, Chemistry, and Mathematics

Publications

I am the corresponding author in my first author publications.

9. Electronic structure, defect stability, and excitonic optical response in $RbTlCl_3$ perovskite solar cells: A first-principles study

Siddharth, **Vinod Kumar Solet**, and Sudhir K. Pandey https://arxiv.org/abs/2508.16264 (Under review)

8. Significant first-principles electron-phonon coupling effects in the LiZnAs and ScAgC half-Heusler thermoelectrics

Vinod Kumar Solet and Sudhir K. Pandey, Phys. Rev. B **113**, 115203 (2026).

7. Many-body *ab initio* study of quasiparticles, optical excitations, and excitonic properties in LiZnAs and ScAgC for photovoltaic applications

Vinod Kumar Solet and Sudhir K. Pandey, Phys. Rev. Applied **23**, 064040 (2025).

6. Understanding the transport behavior of PbSe: A combined experimental and computational study

Isha Sihmar, Abhishek Pandey, **Vinod Kumar Solet**, Neeru Chaudhary, Navdeep Goyal and Sudhir K. Pandey, Next Materials **8**, 100702 (2025).

5. Band gap renormalization, carrier mobility, and transport in Mg_2Si and Ca_2Si: *Ab initio* scattering and Boltzmann transport equation study

Vinod Kumar Solet and Sudhir K. Pandey, Phys. Rev. B **111**, 205203 (2025).

4. Probing the magnetic ground state of stretched diamond lattices $NaTaO_4$ and $NdNbO_4$: Impact of spin-orbit coupling and crystal electric field

Jogendra Kumar, **Vinod Kumar Solet**, Dheeraj Ranaut, Sudhir K. Pandey and K. Mukherjee, J. Phys.: Condens. Matter **37**, 135803 (2025).

3. Mg_2Si and Ca_2Si semiconductors for photovoltaic applications: Calculations based on density-functional theory and the Bethe-Salpeter equation

Vinod Kumar Solet and Sudhir K. Pandey, Phys. Rev. Applied **22**, 064060 (2024).

2. Ab initio study of phononic thermal conduction in ScAgC half-Heusler

Vinod Kumar Solet and Sudhir K. Pandey, Eur. Phys. J. B **96**, 53 (2023).

1. First-principles study of optoelectronic and thermoelectronic properties of the ScAgC half-Heusler compound

Vinod Kumar Solet, Shamim Sk, and Sudhir K. Pandey, Phys. Scr. **97**, 105711 (2022).

Peer Reviewer

- Journal of Physics D: Applied Physics, Physica Scripta, ACS Omega, Bulletin of Materials Science, Materials Research Express, Journal of Modern Physics

Conference and Workshop

- Selected in a poster presentation at the "Joint ICTP MARVEL College: Materials simulations in the age of AI and 2026 School on Electron-Phonon Physics and Many-body Perturbation Theory", Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy (1-21 June 2026)
- Participated in a poster presentation at the "Yambo School on Many-Body Perturbation Theory and Excited-State Simulations", University of Modena and Reggio Emilia, Modena, Italy (19–23 May, 2025)
- Participated in a poster presentation at the "International Conference on 60 Years of DFT: Advancements in Theory & Computation", IIT Mandi, India (21-26 July 2024)
- Participated in a poster presentation at the CECAM Flagship school on "Theoretical Spectroscopy Lectures", EPFL, Switzerland (11–15 March, 2024)
- Participated in a poster presentation at the "34th AGM of MRSI and 5th Indian Materials Conclave", IIT(BHU), India (12–15 Dec, 2024)
- Online participation in the "2023 Virtual School on Many-body Calculations using EPW and BerkeleyGW", UT, USA (5-9 June, 2023)

Teaching Assistant (TA) at IIT Mandi

- Quantum Mechanics for Material Science (MT-XX2), Fall semester 2024
- Computational Methods in Material Science (EN-511), Spring semester (2023 and 2024)
- Functional Materials for Energy Engineering (EN-509), Fall semester 2022
- Electromagnetic Theory (PH-521), Spring semester 2022
- Mathematical Physics and Engineering Mathematics-2 (PH-511 and EP-301), Fall semester 2021

Awards and Achievements

- ANRF International Travel Grant (2025)
- MCM Scholarship, IIT Mandi
- CM Higher Education Scholarship 2015-2018
- Qualified JEST, GATE, IIT-JAM

Personal Details

- Language: English, Hindi
- Date of Birth: February 05, 1997
- Permanent Address: VPO.- Giruri, Teh.- Bansur, Dist.- Kotputli-Behror, Rajasthan, India