Suhas Nahas

Contact Information

216A, Old R.A Hostel, IIT Kanpur
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Research Interests

- Group theory in condensed matter physics
- Topological insulators, 2D materials and Dirac-Fermionic materials
- Electron correlations and magnetism in materials
- Algorithms for abinitio thermodynamics : cluster expansion, simulated annealing/quenching and evolutionary algorithms

Education

Indian Institute of Technology, Kanpur.

- M Tech, *Materials Science and Engineering*, May 2015. **GPA** : 9.5/10

National Institute of Technology, Calicut.

- B Tech, *Mechanical Engineering*, May 2013. **GPA** : 7.0/10

St. Antony's Public School, Kottayam.

- Std XII, *AISSCE*, March 2009. **Score** : 90.0/100

Infant Jesus Higher Secondary School, Kollam.

- Std X, *ICSE*, March 2007. **Score** : 90.7/100

Work Experience

09/2015 - present :

- Project Engineer, *Computational Materials Science Lab*, IIT Kanpur

Postgraduate Research

- **Dissertation:** A computational study on predicting the structure of amorphous semiconductors using evolutionary algorithms
- Electric field induced gap modification in ultrathin blue phosphorous
- Chemical functionalization of black phosphorene
- Polymorphism in phosphorene and arsenene using evolutionary algorithms

Undergraduate Research

- **Dissertation:** Graphene reinforcement on metal and polymer matrices

Refereed Journal Publications

- **Nahas, S.**; Ghosh, B.; Bhowmick, S.; Agarwal, A. "First-Principles cluster expansion study of functionalization of black phosphorene via fluorination and oxidation" – Phys. Rev. B (2016)
- Ghosh, B.; **Nahas, S.**; Bhowmick, S.; Agarwal, A. "Electric field induced gap modification in ultrathin blue phosphorus" – Phys. Rev. B (2015)

Submitted Journal Publications

- **Nahas, S.**; Gaur, A.; Bhowmick, S. "First-Principles prediction of amorphous phases using evolutionary algorithms"

Papers in Preparation

- **Nahas, S.**; Bajaj, A.; Bhowmick, S. "New polymorphs of phosphorene and arsenene"

Relevant Courses

- Electronic structure of materials
- Computational materials science
- Nanostructures and nanomaterials
- Symmetry and tensor properties of materials
- Mathematics and computational methods
- Transport phenomena
- Thermodynamics of materials
- Structure and characterization of materials

Research Skills

- ***Electronic Structure Codes***:
  - ⇒ **VASP & Quantum Espresso**: Density functional theory, Hybrid functionals, Density functional perturbation theory (Phonons) and Abinitio molecular dynamics (CPMD & BOMD)
  - ⇒ **BerkeleyGW**: Quasi-particle Energies based on GW approximation, Dielectric matrix and Optical Responses.
  - ⇒ **CASINO**: Variational monte-carlo, Diffusion monte-carlo
- ***First-Principles Thermodynamics Codes***:
  - ⇒ **Universal Structure Prediction Xtallography**: Evolutionary algorithms for predicting stable/metastable phases from *first principles* in all dimensions and transition pathways between different phases.
  - ⇒ **MIT Abinitio Phase Stability**: Cluster Expansion for determining the stability of alloys and defects from *first principles*
  - ⇒ **Eazy Monte Carlo Code**: Determining the entire phase diagram for varying compositions of alloys and defects from from *first principles*
- ***Basic Computational Skills***:
  - ⇒ **Programming Languages**: Fortran, Python
  - ⇒ **Scripting Languages**: BASH
  - ⇒ **Numerical Computing Tools**: R, MATLAB
  - ⇒ **Typesetting Tools**: LaTeX, Microsoft Office
  - ⇒ **Plotting Tools**: Gnuplot, Matplotlib
  - ⇒ **Operating Systems**: Linux, Windows

International Workshops

- **S N Bose - JAIST School on Quantum Monte Carlo** Mar, 2015
  - ⇒ Hands-on training in CASINO code
  - ⇒ Talks on the theoretical developments of Quantum Monte Carlo
- **8^{th} USPEX Workshop** Jan, 2015
  - ⇒ Hands-on training in Universal Structure Prediction Xtallography code
  - ⇒ Talks on the modern methods of crystal structure prediction

References

Dr. Somnath Bhowmick
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