Pinku Nath, Ph.D

Scientific Software Developer
Phone: (+91) 8472-075908
Email: pinkunath09@gmail.com
web-link :tap-here

Software Developer

Primary developer of AQHA (link, link)
AQHA is a python wrapped C++ based ab-initio High-throughput software. It efficiently computes thermodynamic, mechanical and transport properties. This package is equally efficient to incorporate strong anharmonic effects which plays a significant role in computing material properties accurately at high-temperature. An objective of this project is to accelerate the discovery of ultra-high temperature materials. It will soon be available with GPL-licence.The package uses QHA3P-methodology, an accelerated quasi-harmonic technique developed by me. It reduces huge computational cost without compromising accuracy.

A developer of AFLOW (link)
AFLOW is a C++ based ab-initio High-throughput software.

Primary developer of kMC-Heteroepitaxy code (link, link)
It is a code written in C parallel with Open-MPI which allows to study surface morphology of hetero-epitaxial thin film growth. Due to different natures of film and substrate materials, lattice strain develop at the interface which governs the morphology of the grown thin films. Ball and spring model has been used to simulate lattice strain. Effects such as temperature, rate of deposition and annealing are modelled using kinetic Monte Carlo technique.

Assistant Professor

Lovely Professional University, Jalandhar-144411, Punjab, India 2019-2021
School of Chemical Engineering and Physical Sciences.
Teaching, Research and Organizing workshops (link).

Postdoctoral Associate

Pratt School of Engineering, Duke University, Durham, NC-27705 2014-2019
School of Chemical Engineering and Physical Sciences.
Involved in developing scientific software within AFLOW, a C++ based high throughput software, for computing various kind of materials properties such as electronic, thermal, mechanical, stability and many others. (link)

Ph.D

Computational Chemistry 2006-2014
IIT-Kanpur, India.
Thesis: *Kinetic Monte Carlo Simulations of Growth of Hetero-epitaxial Thin Films*

M.Sc

Chemistry 2004-2006
IIT-Guwahati, India.
Project: *Vanadium-Catalyzed Selective Oxidation of Alcohols to Aldehydesand Ketones with tert-Butyl Hydroperoxid*

Skills

C, C++	Expert level
Open MPI	Expert level
Python	Expert level
SQL	Intermediate level
Machine Learning	Expert level

Expertise

Stochastic methods	Monte carlo, kinetic Monte Carlo, evolutionary algorithms
Electronic Structure Theory	Hartree-Fock method, DFT
Molecular Dynamics	

Expertise in commercial SOFTWARE CODES

VASP	A package to perform electronic structure calculations.
Quantum-Espresso	A package to perform electronic structure calculations.
ATAT	A method to compute phase diagram, structural stability *etc.*
LAMMPS	It is a classical molecular dynamics code.
USPEX	It is a code for predicting the structure of crystals, surfaces and nanoparticles.

Publications

1. **P. Nath**, J. J. Plata, J. Santana, E. J. Blancas, A. M. Márquez, J. F. Sanz, *"High-throughput screening of the thermoelastic properties of ultra-high temperature ceramics"*. **ACS Appl. Mater. Interfaces**, 13, 29843–29857, 2021. (link)

2. J. R. Choudhuri, **P. Nath**, *"Wetting Transition of a nanodrop on switchable hydrophilic-hydrophobic surfaces"*, **Surf. Interfaces** 21, 100628, 2020.(link).

3. A. Singh, J. C. Mehta, D. Anand, **P. Nath**, B. Pandey A. Khamparia, *"An intelligent hybrid approach for hepatitis disease diagnosis: Combining enhanced k-means clustering and improved ensemble learning"*, **Expert Systems**, e12526, 2020. (link).

4. A. Singh, **P. Nath**, V. Single, D. Anand, Kavita, S. Verma, T. P. Hong, *"A New Clinical Spectrum for the Assessment of Nonalcoholic Fatty Liver Disease Using Intelligent Methods"*, **IEEE Access**, 138470, 8, 2020. (link).

5. K. S. Maan, A. Sharma, **P. Nath**, Dai-Viet N. Vo, Hoang Thu Ha, T. D. Minh, *"Application of carbon-based smart nanocomposites for hydrogen production: current progress, challenges, and prospects"*, **Elsevier, a book chapter**, 2020, ISBN: 9780128195536. (link).

6. **P. Nath**, D. Usanmaz, D. Hicks, C. Oses, M. Fornari, M. B. Nardelli, C. Toher, S. Curtarolo, *"AFLOW-QHA3P: Robust and automated method to compute thermodynamic properties of solids"*, **Phys. Rev. Mater. 3, 073801, 2019.** (link).

7. D. Usanmaz, **P. Nath**, C. Toher, J. J. Plata, R. Friedrich, M. Fornari, M. B. Nardelli, and S. Curtarolo, *"Superlattices of topological insulators"*, **Chem. Mater.**, 30,2331-2340, 2018. (link).

8. C. Toher, C. Oses, D. Hicks, E. Gossett, F. Rose, **P. Nath**, D. Usanmaz, D.C. Ford, E. Perim, C.E. Calderon, J.J. Plata, Y. Lederer, M. Jahnatek, W. Setyawan, S. Wang, J. Xue, K. Rasch, R.V. Chepulskii, R.H. Taylor, G. Gomez, H. Shi, A.R. Supka, R. Al Rahal Al Orabi, P. Gopal, F.T. Cerasoli, L. Liyanage, H. Wang, I.

Silo, L.A. Agapito, C. Nyshadham, G.L.W. Hart, J. Carrete, F. Legrain, N. Mingo, E. Zurek, O. Isayev, A. Tropsha, S. Sanvito, R.M. Hanson, I. Takeuchi, M.J. Mehl, A.N. Kolmogorov, K. Yang, P. D'Amico, A. Calzolari, M. Costa, R. De Gennaro, M. Buongiorno Nardelli, M. Fornari, O. Levy, and S. Curtarolo. *"The AFLOW Fleet for Materials Discovery"*, Handbook of Materials Modeling. pp. 1-28 Springer, Cham (2018), a book chapter, ISBN 978-3-319-44677-6 (link).

9. J. J. Plata, **P. Nath**, D. Usanmaz, J. Carrete, C. Toher, M. de Jong, M. D. Asta, M. Fornari, M. B. Nardelli, and S. Curtarolo, *"An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOW-AAPL Automatic Anharmonic Phonon Library"*, **NPJ Comput. Mater.**, 45, 2017 (link).

10. **P. Nath**, J. J. Plata, D. Usanmaz, M. Fornari, M. B. Nardelli, C. Toher, and S. Curtarolo, *"High Throughput combinatorial method for fast and robust prediction of lattice thermal conductivity"*, **Scripta Mater.**, 129, 88-93, 2017 (link).

11. **P. Nath**, J. J. Plata, D. Usanmaz, R. Al Rahal Al Orabi, M. Fornari, M. B. Nardelli, C. Toher, and S. Curtarolo, *"High-Throughput Prediction of Finite-Temperature Properties using the Quasi-Harmonic Approximation"*, **Comp. Mat. Sci.**, 125, 82-91, 2016 (link).

12. D. Usanmaz, **P. Nath**, J. J. Plata, Gus L. W. Hart, I. Takeuchi, M. B. Nardelli, M. F. and S. Curtarolo, *"First principles thermodynamical modeling of the binodal and spinodal curves in lead chalcogenides"*, **Phys. Chem. Chem. Phys.**, 18, 5005, 2016 (link).

13. P. Ghosh, **P. Nath**, M. Ranganathan, *"Understanding the early stages of growth of Ge on Si(001) from lattice based simulations"* **Surf. Sci.**, 639, 96, 2015 (link).

14. **P. Nath**, M. Ranganathan, *"Study of Stranski–Krastanov growth using kinetic Monte Carlo simulations with an atomistic model of elasticity"*, **Surf. Sci.**, 628, 8, 2014 (link).

15. **P. Nath**, M. Ranganathan, *"Kinetic Monte Carlo simulations of heteroepitaxial growth with an atomistic model of elasticity"*, **Surf. Sci.**, 606, 1450, 2012 (link).

16. L. Rout, **P. Nath**, T. Punniyamurthy, *"Vanadium-Catalyzed Selective Oxidation of Alcohols to Aldehydes and Ketones with tert-Butyl Hydroperoxide"*, **Adv. Synth. Catal.** 349,846, 2007 (link).

Selected Presentations:

1. **P. Nath**, J. J. Plata, D. Usanmaz, M. B. Nardelli , M. Fornari , S. Curtarolo, Strong negative thermal expansion in metal carbides using the quasi-harmonic approximation, **APS March Meeting, New Orleans, Louisiana** 2017, Abstract: L8.00010.

2. **P. Nath**, Jose J. Plata , Cormac Toher , Stefano Curtarolo, High-throughput thermodynamics of vibrational degrees of freedom with AFLOW. **APS March Meeting** 2015, Volume 60, Number 1.

3. **P. Nath** and M. Ranganathan, Kinetic monte carlo simulattions of thin film growth: **Symposium on HPC Applications**, march 12-14 (HPC-2012).(poster presentations).

4. **P. Nath** and M. Ranganathan, Kinetic Monte Carlo Simulations of growth of heteroepitaxial thin films: **Theoretical Chemistry Symposium** (TCS-2010). IIT-Kanpur, India. 8-12 December, 2010.(Poster presentation).

5. **P. Nath** and M. Ranganathan, Kinetic Monte Carlo Simulations of growth of heteroepitaxial thin films: Thin Films and Crystal Growth Mechanisms. **Gordon Research Conferences**, at University of New England in Biddeford ME United State from 07/16/2011 - 07/17/2011 (GRC-2011).(Poster presentation).

Journal Reviewed

1. A reviewer of Journal of Computational Electronics (link)

Awards and Honors:

- Carl Storm International Diversity Fellowship for attending Gordon Research Conference, **2011**
- Graduate Research Fellowship from Council of Scientific & Industrial Research, **2007-2011**
- Best Poster Award in Theoretical Chemistry Symposium, **2010**