MADHUBANTI MUKHERJEE

SCIENTIST, EPFL,

SWITZERLAND

CONTACT

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SKILLS

- **OS:** Linux (ubuntu), MS office
- **Programming languages:** Python (with expertise in ML libraries), MATLAB, BASH
- **High Performance Computing**
- **Modeling and simulations:** VASP, Quantum Espresso, WIEN-2K, LAMMPS, Phonopy, Phono3py, ShengBTE, AlmaBTE, BoltzTraP, TDEP, USPEX, Pymatgen, ASE
- **Machine learning:** Supervised learning, deep learning, predictive modeling, feature engineering and selection, model evaluation and validation, teamwork through Git
- **Graphics:** Adobe illustrator and Inkscape
- **Plotting tools:** XMgrace, GNUplot, Plotly, Matplotlib, Seaborn
- **Visualization tools:** CrystalMaker, VESTA, VMD, and p4vasp
- Scientific writing
- Project Coordination

PROFESSIONAL SUMMARY

Computational materials scientist with a Ph.D. from the Indian Institute of Science, Bangalore, India. My research focuses on designing materials for energy applications, leveraging density functional theory, molecular dynamics, and machine learning. I am proficient in using different programming languages such as Python, MATLAB, and have experience with bash scripting. I am well-versed with graphical designing suits.

RESEARCH INTERESTS

- Density functional theory, Molecular dynamics
- Electronic structure properties of materials, thermoelectric, dielectric, mechanical, piezoelectric, electronic, and thermal transport properties of organic and inorganic materials across all length scales
- Device level challenge for materials and additive manufacturing
- High-throughput screening, and machine learning

EXPERIENCE

November 2024 - Present

Scientist

LCBC, EPFL

- Designing perovskites for solar cell applications
- Designing systems for molecular electronics applications

October 2021 – August 2024

Postdoctoral Research Associate

School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta

- Developing and implementing computational models to analyze research data and interpret results
- Collaborating with colleagues to develop new methodologies for research projects
- Compiling and assisting in preparing reports for granted research projects
- Presented findings at conferences and published papers in peer-reviewed journals

LINGUISTICS

- English
- Hindi
- Bengali

ACHIEVEMENTS AND AWARDS

a. I got selected as a participant in the 2024 Leadership and Management in Action Program (L-MAP) at Georgia Tech.

b. Recipient of the prestigious INSPIRE SHE scholarship (2010-2015) awarded by the Department of Science and Technology.

c. Recipient of prestigious INSPIRE FELLOWSHIP for Ph.D. (2016), awarded by the Department of Science and Technology.

d. Qualified National Graduate Aptitude Test in Physics (GATE-2016) for Ph.D.

e. **Invited talk:** Breaking Boundaries AI-Driven Design of High-Temperature Polymer Dielectrics (Annual SPN Symposium, Georgia Tech 2024)

PROFESSIONAL PROFILES

Google Scholar

Researchgate

Linkedin

February 2021 - August 2021

Research Associate

Materials Research Centre, Indian Institute of Science, Bangalore

- Providing training on tools used in conducting research projects
- Conducted extensive research to develop innovative solutions for complex problems

EDUCATION

2016 - 2021

Doctor of Philosophy

Materials Research Centre, Indian Institute of Science, Bangalore

2013 - 2015

Master of Science (Physics)

St. Xavier's College, University of Calcutta, Kolkata

2011 - 2013

Bachelor of Science (Physics)

Midnapore College, Vidyasagar University

PUBLICATIONS

Published:

1. **Madhubanti Mukherjee**, George Yumnam, Abhishek K. Singh, "High Thermoelectric Figure of Merit via Tunable Valley Convergence Coupled Low Thermal Conductivity in $A^{II}B^{IV}C^{V}_2$ Chalcopyrites" J. Phys. Chem. C, 122, 51, 29150 (2018)
2. **Madhubanti Mukherjee,** Abhishek K. Singh, "Strong Chemical Bond Hierarchy Leading to Exceptionally High Thermoelectric Figure of Merit in Oxychalcogenide AgBiTeO" ACS Appl. Mater. Interfaces, 12, 7, 8280 (2020)
3. **Madhubanti Mukherjee,** Swanti Satsangi, Abhishek K. Singh, "A Statistical Approach for the Rapid Prediction of Electron Relaxation Time Using Elemental Representatives" Chem. Mater., 32, 15, 6507 (2020)
4. Partha Kumbhakar, Partha Kumbhakar, **Madhubanti Mukherjee,** A. Pramanik, S. Karmakar, Abhishek K. Singh, Chandra Sekhar Tiwary, P. Kumbhakar, "Confinement Aided Simultaneous Water Cleaning and Energy Harvesting Using Atomically Thin Wurtzite (Wurtzene)" Adv. Sustain. Syst., 2000189 (2020)
5. Animesh Bhui, Moinak Dutta, **Madhubanti Mukherjee,** Kewal Singh Rana, Abhishek K. Singh, Ajay Sonic and Kanishka Biswas, "Ultralow

WORKSHOP ATTENDED

1. "Computational methodologies across all length scale", BRNS, BARC Mumbai, India, 2017

2. VASP workshop, "Advanced optics and dielectric properties", 2024

SELECTED PRESENTATION

a. AI and Materials II, APS March Meeting (2023) (Oral presentation) Recent Advances in Data-Driven Discovery of Materials for Energy Conversion and Storage, Materials Research Society (2022)
b. International Conference on Electron-Phonon Coupling and Thermoelectric Efficiency (2020)
c. VCT 2020
d. Thermoelectric materials, APS March Meeting (2020) (canceled due to COVID-19)
e. Thermoelectric Energy Conversion: Complex Materials and Novel Theoretical Methods, Materials Research Society (2019)
f. International Conference on Hybrid and Organic Photovoltaics, Roma, Italy (2025)

thermal conductivity in earth-abundant Cu1.6Bi4.8S8 : anharmonic rattling of interstitial Cu" Chem. Mater., 33, 8, 2993 (2021)

6. P. Kumbhakar, C. C. Gowda, P. L. Mahapatra, **Madhubanti Mukherjee,** K. D. Malviya, M. Chaker, A. Chandra, B. Lahiri, P. M. Ajayan, D. Jariwala, Abhishek K. Singh, Chandra Sekhar Tiwary, "Emerging 2D metal oxides and their applications" Mat. Today 45, 142-168 (2021)

7. Ashutosh Srivastava, **Madhubanti Mukherjee**, Abhishek Kumar Singh, "Decoupled atomic contribution boosted high thermoelectric performance in mixed cation spinel oxides ACo_2O_4" Appl. Phys. Lett. 120, 243901 (2022)

8. **Madhubanti Mukherjee,** Ashutosh Srivastava, Abhishek Kumar Singh, "Recent Advances in Designing Thermoelectric Materials" J. Mater. Chem. C, 10, 12524-12555 (2022)

9. Partha Kumbhakar, Arko Parui, Rushikesh S Ambekar, **Madhubanti Mukherjee,** Saif Siddique, Nicola M Pugno, Abhishek K Singh, Chandra S Tiwary, "Rain energy harvesting using atomically thin Gadolinium Telluride decorated 3D Printed nanogenerator" Adv. Sustain. Syst., 2200296 (2022)

10. **Madhubanti Mukherjee,** Harikrishna Sahu, Mark D. Losego, Will R. Gutekunst, and Rampi Ramprasad, "Informatics-driven Design of Superhard B-C-O Compounds", ACS Appl. Mater. Interfaces, 16, 8, 10372–10379 (2024)

11. Stuti Shukla, Chao Wu, Ankit Mishra, Junkun Pan, Aaron P. Charnay, Ajinkya Deshmukh, Ashish Khomane, Jierui Zhou, **Madhubanti Mukherjee,** Rishi Gurnani, Riccardo Casalini, Rampi Ramprasad, Michael D. Fayer, Priya Vashishta, Yang Cao, Gregory Sotzing, "Pendant Group Functionalization of Cyclic Olefin for High Temperature and High-Density Energy Storage", Advanced Materials, 2402133, (2024)

12. Ashutosh Srivastava, **Madhubanti Mukherjee**, and Abhishek Kumar Singh, "Role of phonon scattering and bonding in resolving lattice thermal conductivity ambiguities of b-Ga_2O_3", Dalton Transactions 53 (38), 16023-16029 (2024)

13. Jing Hao, Irene Mutegi, **Madhubanti Mukherjee**, Harikrishna Sahu, Ashish Khomane, Rampi Ramprasad, Gregory Sotzing, Yang Cao, "High-temperature high-k polyolefin by rational molecular design", Proceedings of the National Academy of Sciences, 121 (50), e2415388121 (2024)

14. Harikrishna Sahu, Mingzhe Li, **Madhubanti Mukherjee**, Liang Yue, H. Jerry Qi, and Rampi Ramprasad, "Elucidating the Photochemical Conversion Mechanism of PDMS to Silica under UV Light and Ozone", J. Phys. Chem. Lett. 16, 3, 747-753 (2025)

15. Jing Hao, Stuti Shukla, Rishi Gurnani, **Madhubanti Mukherjee**, Harikrishna Sahu, Ashish Khomane, Pritish Aklujkar, Mohak Desai, Chao Wu, Rampi Ramprasad, Gregory Sotzing, Yang Cao, "Stereoisomerism of Vicinal Polydichloronorbornene for Ultra-High-Temperature Capacitive Energy Storage", Advanced Materials, 2417625 (2025)

Ongoing Research Activities:

1. **Madhubanti Mukherjee,** Harikrishna Sahu, and Rampi Ramprasad, "Machine learning guided framework for robust hardness prediction"
2. Shivank Shukla[$], **Madhubanti Mukherjee[$]**, Rishi Gurnani, and Rampi Ramprasad, "Informatics Driven Designing of High Temperature Polymer Dielectrics." ([$]Equal contribution)
3. **Madhubanti Mukherjee**, Ashutosh Srivastava, and Abhishek Kumar Singh, "Critical Descriptor to Capture Anharmonicity."
4. **Madhubanti Mukherjee**, Ashutosh Srivastava, and Abhishek Kumar Singh, "High-Throughput Designing of Thermoelectric Interface Materials."