CHIKU PARIDA

Ph.D. Student

Technical University of Denmark - DTU, Lyngby, Denmark

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EDUCATION

Doctor of Philosophy

Technical University of Denmark - DTU April 2023 – March 2026 Denmark

Supervisors: Dr. Arghya Bhowmik, Prof. Juan Maria Garcia Lastra; Department of Energy Conversion and Storage, DTU.
Project Title: 'Deep Generative Models for Inverse Design of Solid Electrolytes'

Post Graduate Diploma in Materials Science

Jawaharlal Nehru Centre for Advanced Scientific Research(JNCASR) September 2021 – August 2022 India

Supervisor: Prof. Shobhana Narasimhan; Professor, Theoretical Sciences Unit, JNCASR.
Project Title: 'First Principles Study of Dissolution of Platinum in Water'.

Master of Science in PHYSICS

Indian Institute of Technology - BHU 2019 – 2021 India

- GPA: 9.44/10
- Thesis: 'Density Functional Theory Study of Topological Materials'.

Bachelor of Science in PHYSICS

Odisha University of Agiculture and Technology 2016 – 2019 India

- GPA: 8.87/10
- Dissertation: 'Designing Class-A Power Amplifier for High Frequency Applications'.

EXPERIENCE

Doctoral Researcher

Technical University of Denmark - DTU April 2023 – Present Lyngby, Denmark

Supervisor: Prof. Juan Maria Garcia Lastra and Dr. Arghya Bhowmik; DTU Energy, DTU.

Projects:
- Inverse design of solid electrolytes and cathodes for Li-ion batteries.
- High-throughput materials discovery using physics informed deep learning models

Exchange PhD Student

Department of ENG., University of Cambride April 2025 – August 2025 Cambridge, United Kingdom

Group: Computational Mechanics; Prof. Gábor Csányi

Project:
- Universal Electrostatic MACE ***(On going)***

Visiting PhD Student

École polytechnique fédérale de Lausanne (EPFL) November 2023 – December 2024 Lausanne, Switzerland

Group: THEOS, EPFL; Prof. Nicola Marzari

Materials Design Intern (Research Engineer)

QPIVOLTA TECHNOLOGIES PVT LTD July 2022 – November 2023 Bangalore, India

Projects:

- High-throughput Discovery of Solid Electrolyte for Na-Ion Batteries.
- Machine Learning Interatomic Potentials for Interfaces.

PGDMS Project Student

Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) Sep 2021 – Aug 2022 India

Supervisor: Prof. Shobhana Narasimhan; Professor, Theoretical Sciences Unit, JNCASR, India.
Collaborator: Dr. Brandon C. Wood; Deputy Group Leader; Quantum Simulations Group, Lawrence Livermore National Laboratory(**LLNL**), U.S.

Projects:
- First Principles Study of Dissolution of Platinum in Water

SKILLS

1. **Python**
   - Statistical simulations, scripting, coding, etc.
2. **Machine Learning(ML)**
   - Development of ML models for materials discovery.
3. **Deep Learning(DL)**
   - Machine Learning Interatomic Potentials (MLIAPs) for chemistry and materials.
   - Deep generative models for inverse design of materials.
4. **Density Functional Theory(DFT) computations using VASP - Vienna Ab initio Simulation Package, Quantum ESPRESSO and Atomic SImulation Environment(ASE) & GPAW**
   - Used for the quantum mechanical study of materials.
   - Coupled with machine learning models for high-throughput discovery of materials.
5. **GitHub and GitLab**
6. **Linux**
7. **LaTeX**

PUBLICATIONS

1. Mining Chemical Space with Generative Models for Battery Materials; **Parida C**, Roy D, Garcia Lastra JM, Bhowmik A; Batteries & Supercaps, p.e202500309 (DOI).
2. Limitations of Foundation Models in Energy Materials Simulations: A Case Study In Polyanion Sodium Cathode Materials; Petersen MH, **Parida C**, Busk J, Garcia Lastra JM, Bhowmik A, 2025, *Under Review*.
3. Element-Specific Neighbor Lists for Periodic Graph Neural Networks; **Parida C**, In AI4X 2025 International Conference.
4. Reflections from the 2024 large language model (llm) hackathon for applications in materials science and chemistry; Zimmermann Y, Bazgir A, Afzal Z, Agbere F, Ai q, Alampara N,.., **Parida C**, Petersen MH,..., Blaiszik B, arXiv preprint arXiv:2411.15221. 2024 Nov 20.
5. A Practical Database for Halide-based Solid electrolytes; **Parida C**, Garcia Lastra JM, Bhowmik A; *Under preparation*.
6. Defect Engineered Li-ion Super Conductors: Enhancing Ionic Conductivity By Vacancies, Dopants and Anti-site Defects; **Parida C**, Bhowmik A, Garcia Lastra JM; *Under preparation*.

ACHIEVEMENTS

- **DFTPilot[2025 Visionary Award]:**LLM Hackathon for Applications in Materials Science and Chemistry (GitHub)
- **E-Resources Grant (H2-2024 Opslag af regnetid på nationale e-ressourcer):** The grant covers 3 million CPU-core-hours, and 250K GPU-core-hours with 350K TB-hours of computational resources on LUMI supercomputer issued by the Danish e-Infrastructure Consortium (DeiC).
- **Invited Talk:** Defect Engineered Solid Electrolytes and Cathodes for Li-ion Batteries; Nanyang Technological University **(NTU)**/A*STAR Institute of Materials Research and Engineering **(A*STAR IMRE)**, Singapore, 2025
- **Oral Presentation:** AI-assisted Inverse Design of Solid Electrolytes (Modeling Disorders!); 12th International Conference on Materials for Advanced Technologies **(ICMAT - 2025)**, Singapore, 2025

LANGUAGES

English **Hindi** **Odia**
Mother tongue

ACADEMIC REFEREES

Prof. Juan Maria Garcia Lastra
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