RIBHU BHATIA

ABOUT ME

I am currently a Doctoral Candidate in the Department of Chemical Sciences at University of Ferrara, specialising in computational chemistry with focus on energy materials. My research centres on investigating the electronic structure at the interfaces between solar cell absorber and the charge transport materials, particularly lead halide perovskites, perovskite inspired materials and various transport layers, using Density Functional Theory (DFT). By advancing theoretical understanding of different interfacial interactions, my work contributes to establishing a fundamental framework for designing efficient next generation solar cells.

RESEARCH INTERESTS

Computational Chemistry

Solar Energy Conversion and Storage

Interface Physics

Heat Transfer

EDUCATION

[2022 – Current]
PhD in Chemical Science

I have been investigating the role of interfaces between perovskites/inspired materials and various charge transport layers, using Density Functional Theory (DFT)

[18/09/2018 – 22/07/2022]
Master of Science in Energy Engineering specialising in Power Production from Politecnico di Milano

[10/06/2014 – 10/03/2018]
Bachelor of Technology in Aerospace Engineering from SRM University

WORK EXPERIENCE

University of Ferrara – Ferrara, Italy

City: Ferrara | **Country:** Italy
Doctoral Candidate

[2022 – Current]

- **Investigated the electronic structure of the interface between BiOI, a potential two dimensional absorber for indoor photovoltaics and ZnO, the electron transport layer via DFT.**
- Investigated electronic structure of 3D/2D double perovskite for indoor photovoltaic application.
- Currently investigating structure and electronic property relation in halide perovskites across different crystal facets to elucidate their role on charge dynamics.
- Conducting studies on interface between hybrid halide perovskites facets and different hole transporting materials to advance understanding of charge transfer mechanisms.

University of Porto – Porto, Portugal

City: Porto | **Country:** Portugal
Research Mobility

[01/06/2025 – 07/09/2025]

Fabricated and conducted experimental investigations on the effect of different passivants on the performance of hybrid halide perovskites, extending the work to solar cells with a 3D/2D/carbon electrode configuration as a cost-effective and stable alternative to conventional hole-transport materials and gold contacts. The ongoing analysis of experimental results will be complemented by Density Functional Theory (DFT) calculations to elucidate the interactions between selected passivants and hybrid perovskite facets.

Politecnico di Torino – Turin, Italy

City: Turin | **Country:** Italy

Master Thesis Student

[2021 – 2022]

Title- Evaluating the effect of wettability of the evaporation rate of a sessile droplet.
Summary- I systematically carried out molecular dynamics simulations in a pseudo 3D system containing Lennard- Jones particles. **Equilibrium contact angles and evaporation rates** of nano droplet on heated hydrophobic and hydrophilic substrates were evaluated.

Politecnico di Torino – Turin, Italy

City: Turin | **Country:** Italy

Research Intern

[2019 – 2020]

Analyzed the **electromagnetic shielding effectiveness of a composite material**, as a part of **SMARTFAN European project**. Simulations were performed using COMSOL MULTIPHYSICS to understand the effect of parameters viz. conductivity, thickness, frequency etc. on shielding effectiveness of a composite material.

Fondazione Eni Enrico Mattei (FEEM) – Milan, Italy

City: Milan | **Country:** Italy

Research Intern

[2019 – 2020]

Conducted a comprehensive **Value Chain Analysis** of agricultural crops (Tomato and Cashew) for Okuafo Pa project, a pilot initiative of **ENI's Africa Program**, using data collected through in person fieldwork.

E2-Koncept Sofware Solutions – Bangalore, India

City: Bangalore | **Country:** India

Student Trainee

[06/2015 – 09/2015]

Contributed to the design of a Horizontal Stabilizer using CATIA V-5 for a project from Hindustan Aeronautics Limited (HAL).

PUBLICATIONS

[2024]

Improved Hole Extraction and Band Alignment via Interface Modification in Hole Transport Material-Free Ag/Bi Double Perovskite Solar Cells Through the 2D/3D interface modification we proved that charge recombination is suppressed, and band alignment is improved at the perovskite/CBE interface. In addition, we showed that thickness of the 2D layersenhances the probability for holes in $Cs_2AgBiBr_6$ to be located close to the perovskite/CBE interface, further supporting their extraction. Overall, the PCE of the HTM-free solar cells is improved through the implementation of a low-cost and end-of-waste fabrication strategy.

Journal Name: Solar RRL | **Publisher:** Wiley

[2023]

Heavy pnictogens-based perovskite-inspired materials: Sustainable light-harvesters for indoor photovoltaics In this review we showed that the potential of perovskites inspired materials will play a crucial role in the future market of self-powering IoT devices, which will become a large class of devices in the electronics industry.

Journal Name: APL Energy | **Publisher:** American Institute of Physics (AIP)

[2019]

Enclosure Phenomenon in Varying Forced Flow Convection Work was an attempt to pact optimization of perforated enclosures for internal natural convection heat transfer. Heat dissipation effect is experimented over a flat plate and implications were understood with variation in convective heat transfer coefficient. Controlling parameters viz., plate orientation, perforation shape and size, enclosures in diverse configurations were varied systematically aiming enhanced heat transfer.

Journal Name: ASME 2019 Gas Turbine India Conference

[2019]

Convonics: Acoustics Field Assisted Confined Natural Convective Heat Transfer The work focused on investigating the interaction between acoustic fields and confined free convective heat transfer, with the aim of optimizing acoustic effects to address heat transfer challenges in engineering applications.

Journal Name: Proceeding of 14th International Conference of Heat Transfer, Fluid Mechanics and Thermodynamics.

[2018]

Experimental Investigation of Perforated Enclosures in Confined Natural Convection Systematic experimentation was carried out on forced convection heat transfer apparatus under varying non-linear flow conditions to understand heat transfer, with the purpose of enhancing performance of numerous engineering applications.

Journal Name: ASME 2017 Gas Turbine India Conference

[2017]

Flexible Landing System for Exploration of Rocky Celestial Bodies Through proper design and analysis, the requirements and effectiveness of flexible landing systems for space crafts were explored. Impact stresses developed at the time of landing were analysed for different types of system configurations to determine their applicability and extent of variability. The role of controlling parameters viz. the shape and size of the components, weight of the space craft, materials suitable for building the system etc. under different environmental conditions were probed and optimized for a wide range of terrains.

Journal Name: 68th International Astronautical Congress

[2016]

Enclosure Phenomena in Confined Natural Convection Through proper experimentation, the role of an external enclosure on confined natural convective heat transfer on a square flat plate is explored. The effect and the extent of effect of different external enclosure on heat transfer rates is investigated.

Journal Name: American Journal of Engineering Research (AJER)

MANUSCRIPTS IN PREPARATION

Photoelectron Extraction in BiOI

This work sheds light on the atomistic origins of limited photo conversion efficiency of the BiOI/ZnO based photovoltaic devices and offer design principles to engineer more efficient interfaces.

[Current]

Evaluating the performance of hole transport material over different crystal facet for hybrid valid perovskites materials.

DFT calculation were performed to evaluate the role of facets and hole transport material on charge carrier dynamics.

[Current]

Relationship between the atomic and electronic structure across various crystal facets in hybrid halide perovskites.

I carried out DFT calculations four types of crystal facets, varying chemical composition in all the four cases to establish a structure-property relation which is still unknown.

Lead-free perovskites and derivatives for photogeneration: a roadmap to sustainable approaches for photovoltaics and photo(electro)catalysis

This roadmap provides a comprehensive overview of the latest advancements in lead-free perovskite materials for photovoltaic (PV) and photoelectrochemical (PEC)/photocatalytic (PC) applications. It highlights the urgent need for sustainable energy solutions, emphasizing the role of lead-free perovskites in addressing challenges related to toxicity, scalability, and efficiency. The document explores key material families, including tin-, bismuth-, antimony-, copper-, and germanium-based perovskites, detailing their optoelectronic properties, fabrication techniques, and application potential.

PROJECT FUNDING AND PATENTS

[2024 – 2025]

ISCRA class B grant for "Heavy pnictogens based perovskite-inspired materials for indoor photovoltaics(HAPPI)" project

Awarded **1.6 million CPU core hours** on **LEONARDO B**, Cineca's national high-performance computing facility. This competitive allocation enabled large-scale DFT calculations and advanced data analysis. The project was developed in collaboration with Prof. Teresa Gatti from Politecnico di Torino and Prof. Antonio Agresti from the CHOSE lab, of University Roma2 within the context of the **PRIN-PNRR PINPOINT project.**

[2024 – 2024]

ISCRA class C grant for "Effect on vacancy migration due to Halogen bonding at grain boundary in Halide perovskite (EHH)" project

EHH was allocated a total of **160,000 CPU hours** which were used to improve understanding of the halogen bond at the grain boundaries in halide perovskites. More specifically with halogen bonds at perovskites surface, I tracked vacancy migration, which will consequently helped with the estimation of the changes in recovery times.

[2023 – 2024]

ISCRA class C grant for "Optimizing the performance Of facets in multi cation/halide Perovskite Solar cells(OOPS)" project

The **42,000 CPU hours** allocated helped me identify the top performing facet of MAxFA(1-x)PbI(1-y)BRy (FA-formamidinium, MA-methylammonium)-based perovskite.

[01/08/2024 – 06/02/2025]

National Design Patent - Rechargeable Automated Tissue Stainer

The Hematoxylin and Eosin stain is the gold standard in histopathology, but the existing manual and automatic staining methods were either time-consuming or costly and environmentally unsustainable. To address this gap, we proposed a compact, cost-effective, and eco-friendly green autostainer for efficient H&E staining.

CONFERENCES AND SEMINARS

[15/04/2024 – 17/04/2024] Frieburg, Germany

PhD School on Perovskite PV, a joint collaborative effort by DIAMOND and TESTARE Horizon Projects Presented the poster based on my work on the HTM and gold electrode free, carbon based double perovskite cell. Highlighted advances in sustainable, low-cost device architectures suitable for indoor energy harvesting.

[12/06/2024 – 12/06/2024] Ferrara,Italy

1 st PhD Symposium of Chemical Sciences Delivered an oral presentation regarding my work on understanding the role of 2D layers on 3D perovskite, in managing various vacancy and antisite defects in perovskites inspired material.

[19/12/2022 – 19/12/2022] Bologna, Italy

XXIII Emilia Romagna Chemistry Day 2024 Presented a poster regarding stability issue of perovskites solar cells in space. Discussed degradation mechanism and strategies to enhance device resilience in harsh space environment.

[2019 – 2019] Madras, India

ASME 2019 Gas Turbine India Conference, IIT MADRAS Discussed my work via oral presentation, on understanding the role of controlling parameters viz., hot plate orientation, perforation shape and size etc on forced convective heat transfer.

[2017 – 2017] Bangalore, India

ASME 2017 Gas Turbine India Conference Delivered an oral presentation regarding the implications of perforation shape, size and number on natural convection over a hot plate.

[2017 – 2017] Adelaide, Australia

68th International Astronautical Congress Discussed our work on how flexible landing systems for space crafts can expand exploration on rough terrains, via and oral presentation.

PROJECTS

[19/12/2016 – 20/04/2017]

Designed and fabricated a tube stored retractable wing aircraft fro AIAA Design build and Fly competition Designed our unmanned aerial vehicle (UAV) and the Launch Tube to minimize system weight while maximizing speed, range, endurance, storage space and payload capacity thus yielding a minimal Rated Aircraft Cost (RAC).

[06/07/2015 – 07/12/2015]

Contributed to the design and fabrication of a weather monitoring non-autonomous quad copter

SKILLS

Microsoft Word / Microsoft Excel / Microsoft Powerpoint / Microsoft Office / LaTeX

Engineering Design and Simulation

CATIA / AutoDESK AutoCAD (Optimal Knowledge) / ANSYS WORKBENCH , ANSYS FLUENT / OVITO / Moltemplate / Comsol Multiphysics / Classical Molecular Dynamics / VMD / AmberTools / Vesta / VASP / Atomistic simulations using Large-scale AtomicMolecular Massively Parallel Simulator (LAMMPS)

Post Processing Tools

Linux / Fortran / Python / Gnuplot

LANGUAGE SKILLS

Mother tongue(s): Hindi

Other language(s):

Punajbi

LISTENING B2 **READING** A2 **WRITING** A1

SPOKEN PRODUCTION A1 **SPOKEN INTERACTION** A2

English

LISTENING C2 **READING** C2 **WRITING** C2

SPOKEN PRODUCTION C2 **SPOKEN INTERACTION** C2

Italian

LISTENING A1 **READING** A1 **WRITING** A1

SPOKEN PRODUCTION A1 **SPOKEN INTERACTION** A1

German

LISTENING A1 **READING** A1 **WRITING** A1

SPOKEN PRODUCTION A1 **SPOKEN INTERACTION** A1

Marathi

LISTENING C1 **READING** C1 **WRITING** C2

SPOKEN PRODUCTION B2 **SPOKEN INTERACTION** B2

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

AUTHORIZATION

Permission

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