Indian Institute of Technology Delhi

School of Interdisciplinary Research (SIRe)

SIRe Project Number

2022-01-34

(will be assigned by SIRe)

PhD Project

Project Details	
Project Title	**Computational investigation of emerging inorganic and hybrid materials for optoelectronic applications**
Project Summary	The ever-growing energy demand of the world can be met sustainably by using renewable energy sources as well as spending harvested energy most efficiently. In this regard, optoelectronic devices that source, detect, and control photon energy play a major role. These devices are in use for a wide variety of applications ranging from solar cells to light-emitting devices to optical fibers. Despite their potentials, the field of optoelectronics often suffers from a lack of efficient and commercially viable candidate materials as these require several very specific electronic, optical, and transport characteristics. Recently, hybrid halide perovskites have emerged as the next-generation optoelectronic materials. The properties such as suitable optical bandgap, defect-tolerance, fast charge transport, strong absorption coefficients make these materials highly promising. The poor structural stability at operating conditions and the presence of toxic lead, however, pose a serious challenge for the commercialization of halide perovskite-based optoelectronic devices. More recently, fully inorganic halide perovskites appear to be free from short-term stability issues and environment-friendly. Nonetheless, the vast possible chemical space makes it difficult to strategically search and identify the efficient halide perovskites for suitable optoelectronic applications. In this project, we will closely explore one such class of inorganic materials, double halide perovskites. These perovskites have a general formula of $A'A''B'B''X_6$ where A′, A″ are monovalent cations, B′, B″ are monovalent, divalent, or trivalent metals, and X are halogens. The initial computation will vary the chemical components of double perovskites satisfying the valency requirement and generate a large number of candidates. Using several screening criteria, a limited number of potential candidates that have promising electronic and optical properties will be down-selected. To those candidates, we will further employ computationally sophisticated techniques such as many-body perturbation theory and non-adiabatic molecular dynamics to explore the optically excited properties and charge carrier dynamics, respectively. The main deliverable of this project will be to computationally demonstrate a few double halide perovskites with appropriate structural and optoelectronic properties but containing only environmentally non-toxic elements. Scope of the project: (1) To learn density functional theory-based techniques for materials screening for targeted properties. (2) To learn and use non-adiabatic molecular dynamics (NAMD) simulations for studying carrier lifetime and dynamics (3) To learn many-body perturbation theory-based state-of-the-art techniques for estimating the optical properties.

Ph.D. Supervisors			
Role	**Faculty**	**Academic Unit in IITD**	**Email ID**
Supervisor 1	Prof. Dibyajyoti Ghosh	Department of Material Science and Engineering and Department of Chemistry https://mse.iitd.ac.in/faculty-profile/19	dibyajyoti@mse.iitd.ac.in
Supervisor 2	Prof. Saswata Bhattacharya	Physics [https://web.iitd.ac.in/~saswata	saswata@physics.iitd.ac.in

Project requirements (Student qualifications, experience required, etc)

- MSc. / MTech. / Integrated BS-MS in Physics / Chemistry / Materials Science / Materials Engg. / Chemical Engg.
- BTech. in Engineering Physics / Materials Science / Materials Engg. / Chemical Engg.
- Candidates having PMRF / CSIR-UGC NET / GATE / DST Inspire are more encouraged to apply.

Source of funding (IRD/FITT Project details, if any)

1. PMRF/CSIR/UGC/DST Inspire fellowship
2. INSTITUTE fellowship with GATE qualification
3. Any other external funding available at the candidate's end

Role of Faculty Members involved:

The said project contains three parts (1) generating a large number of candidates of double halide perovskites and performing low-cost computation to screen potential candidates (2) Performing non-adiabatic molecular dynamics to study the charge transport characteristics, and (3) Employing many-body perturbation theory-based simulations to understand the optical properties. While the first part is general materials modeling, the latter two parts certainly require expertise in a particular subfield of sophisticated materials modeling.

Here Prof. D. Ghosh and Prof. S. Bhattacharya have extensive experience in computational materials screening. Prof. D. Ghosh further develops and uses cutting-edge NAMD-based techniques to explore the carrier transport properties of semiconductors. Prof. S. Bhattacharya has expertise in theoretical modeling of optical properties using highly accurate many-body perturbation theory-based methods.

Because of these different orthogonal components, this project will be a perfect interdisciplinary theoretical collaboration to fulfill the mentioned research endeavor.