

I-STEM Software Request - Guide Approval Form

User Details

- **Name of Researcher:** Tukadiya Namrata A.
- **User Type:** ☒ Ph.D. Scholar ☐ Postdoctoral Researcher ☐ Bachelor's ☐ Masters
- **Institution Name :** Department of Physics, Faculty of Science, The M. S. U. Baroda, Vadodara
- **Institutional Contact No:** 9429784861
- **Research Topic:** Rational Design of Highly Efficient Solar Cell Materials Using Computational Approach

Software Request Details

- **Software Name:** COMSOL Multiphysics (Basic+Advanced)

Justification for Software Request: My research aims to design and predict high-efficiency solar cell materials, combining machine learning (ML), density functional theory (DFT), and device simulations. COMSOL Multiphysics is essential for achieving my objective computational fabrication and simulation of complete solar cell structures by enabling accurate modeling of the coupled electrical, optical, and thermal behavior within complex multilayered devices. Specifically, COMSOL will allow me to simulate the photovoltaic performance of perovskite, chalcogenide, and chalcopyrite-based solar cells, including the calculation of key parameters such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE). These simulated results will serve as a crucial bridge between material-level predictions (from ML and DFT) and experimental validation, ensuring realistic device design.

Guide/Supervisor Approval

I, Prof. Prafulla Kumar Jha (Guide/Supervisor Name),

- Confirm that the above-mentioned researcher is affiliated with our institution
- Have reviewed the software request and its relevance to the researcher's academic work
- Approve the software request for research purposes

Approval Confirmation

- I approve the software request
- The software aligns with the researcher's research objectives
- The request meets the institutional research guidelines

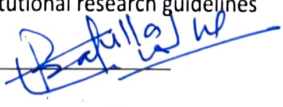
Guide/Supervisor Signature: _____

Date: 29/04/2025

Official Stamp/Seal:

Important Notes

1. This form must be signed and scanned


Prof. Prafulla K. Jha
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