

I-STEM Software Request - Guide Approval Form

User Details

- **Name of Researcher:** Vinay Mirzapure
- **User Type:** [☒] Ph.D. Scholar [☐] Postdoctoral Researcher [☐] Bachelor's [☐] Masters
- **Institution Name:** CSIR- National Chemical Laboratory, Pune
- **Institutional Contact No:** 020- 2590-3140
- **Research Topic:** Developing post Li-ion Energy storage devices.

Software Request Details

- **Software Name:** COMSOL Multiphysics (Basic + Advanced Modules)
- **Justification for Software Request:** [Provide detailed explanation of how the software supports your research objectives]

My research is centered on the development and optimization of post-Lithium-ion energy storage systems, specifically exploring chemistries based on Aluminum, Magnesium, and Sodium. A significant part of this work involves composite electrode materials, optimizing slurries, and developing advanced electrolytes. While synthesizing these materials and evaluating them through physical electrochemical testing protocols, such as galvanostatic charge-discharge cycling, yields essential empirical data, experimental testing alone cannot fully isolate the complex, coupled internal phenomena governing cell performance.

COMSOL Multiphysics is required to bridge this gap between fundamental material synthesis and practical cell behavior. The software will enable the creation of detailed models to simulate the internal electrochemical, transport, and mechanical processes of these emerging battery chemistries.

Specifically, access to the Basic and targeted Advanced Modules will support my research in the following ways:

- **Electrode Architecture Optimization:** Utilizing the **Battery Design and Optimization** modules, we will simulate varying parameters of my composite electrodes to predict the optimal structures for improved capacity and performance.
- **Mitigating Mechanical Degradation:** The insertion of larger or multivalent ions (Na^+ , Mg^{2+} , Al^{3+}) causes severe volumetric expansion in host materials. The **Structural Mechanics Module** will allow us to couple electrochemical kinetics with solid mechanics to predict stress generation, particle fracture, and delamination within the composite electrodes during cycling.
- **Addressing Metal Anode Instability:** For chemistries utilizing metal anodes (such as Zn and Al), dendrite growth and uneven plating are major bottlenecks. The **Electrodeposition Module** is essential for simulating the metal stripping/plating dynamics and localizing current densities to design protective layers and optimized electrolyte formulations.
- **Interfacial and Kinetic Analysis:** The **Chemical Reaction Engineering Module** will facilitate the modeling of complex parasitic reactions, SEI layer formation, and electrolyte transport

properties. This will help interpret the underlying mechanisms behind the fading capacity and impedance growth observed in physical testing.

In conclusion, COMSOL Multiphysics will act as a crucial computational counterpart to my experimental work. It will accelerate material development, reduce experimental waste, and provide the deep mechanistic insights required to optimize these post-Li-ion energy storage systems.

Guide/Supervisor Approval

I, Dr. Manjusha V. Shelke,

- 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: 01/04/2026

डॉ. मनुषा व्ही. शेल्के / Dr. Manjusha V. Shelke
वरिष्ठ प्रभार वैज्ञानिक, भौतिक एवं सामग्री रसायन विज्ञान विभाग
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Official Stamp/Seal: [Space for Institutional Stamp]

Important Notes

1. This form must be signed and scanned
2. The scanned copy must be uploaded with the software request
3. Electronic signatures are acceptable if from an official institutional email