Tata Institute of Fundamental Research
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Internal Webinar

Probing dynamics at the solid-liquid interface in energy materials using NMR spectroscopy and MD simulations

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The performance of any energy storage or conversion device depends on the material's interface and their properties. Therefore, understanding the chemistry at the interface is of fundamental importance in energy materials that find a wide range of applications. It is a challenge to obtain a comprehensive and accurate picture of the structure, dynamics and interactions at the interface. One of the major problems in obtaining a molecular perspective at the interface is to probe only the interfacial species in the presence of a large excess of the bulk species. Nevertheless, nuclear magnetic resonance (NMR) offers various methodologies to access and study these surface or interfacial species, without the interference from the bulk to gain insight at a molecular level. The potential to probe and develop an understanding of the dynamics, interactions and mobility at the solid-liquid interface in nanomaterial dispersions and battery systems using NMR techniques along with molecular dynamics (MD) simulations will be discussed.

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