INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: **ATOMISTIC SIMLATION STUDIES OF ALKALI ION CONDUCTING SUPERIONIC CONDUCTORS**

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SHORT ABSTRACT

All-solid-state batteries, that employs solid electrolytes instead of conventional liquid/gel electrolytes, promises higher energy density, safety and are environmentally benign. The thesis discusses computational investigations on some of the promising classes of Li+/Na+ conducting fast ion conducting solids, that find potential applications in the development of all-solid-state batteries. The study employs state-of-the-art computational techniques such as, classical and ab-initio molecular dynamics (MD), to understand various factors that control ion transport in solids. Some of the salient features of the study are, the role of bottlenecks in the diffusion channels and the significance of the correlated motion of ions with the framework. Further, the thesis discusses a recipe for the efficient implementation of metadynamics (MTD) simulations that accelerates the ion dynamics, there by greatly enhancing the sampling of the phase space and quantification of free-energy landscapes. The efficiency of MTD sampling over standard MD simulation and Nudged Elastic Band (NEB) calculations are critically analyzed.