INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title:		**Molecular Dynamics Investigation of Fast Ion Transport in Oxide Frameworks**
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The thesis reports molecular dynamics(MD) investigation of two families of fast ion conductors, namely, $Na_2M_2TeO_6$, where M=Ni, Zn, Co or Mg, and $Li_{1+x}Ti_{2-x}Al_x(PO_4)_3$, where $0 \leq x \leq 0.67$. These are very promising materials for the development of all-solid-state batteries. Chapter 1 provides a survey of fast ion conduction in various matrices, highlighting complementary knowledge gained through atomistic simulation. Chapter 2 describes the methodology adopted in the present study. Chapter 3 proposes an interatomic-potential-model for $Na_2M_2TeO_6$, where M=Ni, Zn, Co and Mg, where parameters are determined empirically by fitting to the X-ray structure and ionic conductivity reported previously. This chapter also provides fresh insights on the microscopic mechanism of ion transport in these systems. The potential energies and population profiles of the individual Na+ ions mapped on the basal plane suggests entropic contribution playing a significant role in the Na+ transport at the interlayer. A detailed exploration of the role of ion-ion repulsion was carried out in Chapter 4, wherein interlayers of $Na_2Ni_2TeO_6$ having different concentrations of the Na+ ions are examined for their individual self-diffusivity. A comparison of the potential energy and population profiles of Na+ ions for different concentrations demonstrate a gradual cross-over from an energetically driven mechanism (for low concentrations) to an entropically driven mechanism (for high concentrations). It is predicted that an optimal concentration of Na+ ions could improve the ionic conductivity by as much as an order of magnitude. Chapter 5 reports MD study of $Li_{1+x}Ti_{2-x}Al_x(PO_4)_3$, for $0 \leq x \leq 0.67$. For the optimal substitution of Al^{3+} (x=0.33) the Li+ conductivity is found to enhance by two to three orders of magnitude in good agreement with recent experimental results. The study provides fresh insights on the microscopic of ion migration. The conductivity enhancement (for x=0.33) is found to coincide with an increased population of Li+ ions along the Li1-Li1 migration channel, particularly around the Li3 sites. This results in a reduced free-energy barrier for Li+ transport in the system. Chapter 6 summarizes the major findings and conclusions born out of the present MD studies of $Na_2Ni_2TeO_6$, and $Li_{1+x}Ti_{2-x}Al_x(PO_4)_3$.