

Abstract Submitted  
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**Mechanisms of Li-ion transport in bulk electrolytes and through solid-electrolyte interphases (SEI)** DMITRY BEDROV, ZHE LI, University of Utah, OLEG BORODIN, Army Research Laboratory — Performance of Li-ion batteries is strongly coupled to the mechanisms of  $\text{Li}^+$  transport in bulk electrolytes, its transition through electrolyte/SEI interface and its transport through glassy SEI matrix. We will discuss the results of extensive atomistic molecular dynamics (MD) simulations using APPLE&P polarizable force field and that have focused on understanding of correlations between the  $\text{Li}^+$  local structure and the mechanisms of  $\text{Li}^+$  transport in these systems. Specifically, we will address: a)  $\text{Li}^+$  transport in ionic liquid based electrolytes and the influence of organic solvent additives (ethylene carbonate and acetonitrile), b) Li-ion transport through model SEIs comprised of alkyl dicarbonate anions and the influence of SEI contamination by  $\text{Mn}^{2+}$  cations, and c) transition of  $\text{Li}^+$  ions through SEI/electrolyte interfaces.

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