

Abstract Submitted
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Crystalline-amorphous interfaces in Li-ion batteries¹ MARIA K. CHAN, JEFFREY GREELEY, Argonne National Laboratory, CENTER FOR ELECTRICAL ENERGY STORAGE, DOE ENERGY FRONTIER RESEARCH CENTER COLLABORATION — Amorphous and crystalline materials are associated with fast ionic transport and long term structural stability, respectively, both desirable properties in lithium ion battery materials. It is therefore no surprise that amorphous-crystalline interfaces are ubiquitous in Li-ion batteries. Using first principles density functional theory (DFT), and primarily Si as an example, we study models of crystalline-amorphous interfaces in Li-ion batteries. We will discuss the structure of such an interface and its energetic and mechanical effects on lithium insertion, as well as the kinetics of Li ion transport near and across the interface. The mechanism of solid state amorphization will also be discussed.

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Maria K. Chan
Argonne National Laboratory

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