Designing Meaningful Molecular Dynamics (MD) Simulations: The Lithiation of Silicon

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Molecular dynamics (MD) is used to understand the properties of materials by following the time evolution of the system and exploring the interactions between its constituent atoms. MD simulation allows making reliable predictions of various properties of materials; however, designing useful computer experiments is a complex task that requires the appropriate selection of interatomic interactions (force fields) and other conditions. In this work we discuss some aspects of molecular dynamics that would help the inexperienced users design reliable simulations. The simulation of the lithiation process of silicon is taken as an example for better understanding.