Motion and Dynamics of Li in Amorphous SiO

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We investigate the motion and dynamics of a Li atom in amorphous SiO by performing a series of first principles-based atomistic simulations. We perform Monte Carlo simulations to generate realistic SiO structures with varying O-to-Si ratios. Then, we implement a path sampling scheme to obtain detailed thermodynamic information when a Li atom penetrates an SiO matrix. Electronic structure analysis reveals that the thermodynamic stability of a Li atom is determined by local Si-O network environment surrounding Li. The identified thermodynamic information regarding the Li dynamics in SiO provides additional insight into the Li insertion and extraction kinetics in silicon-based Li-ion batteries.