batteries

MDPI

Supplemental Information

Understanding Solid Electrolyte Interphase Nucleation and Growth on Lithium Metal Surfaces

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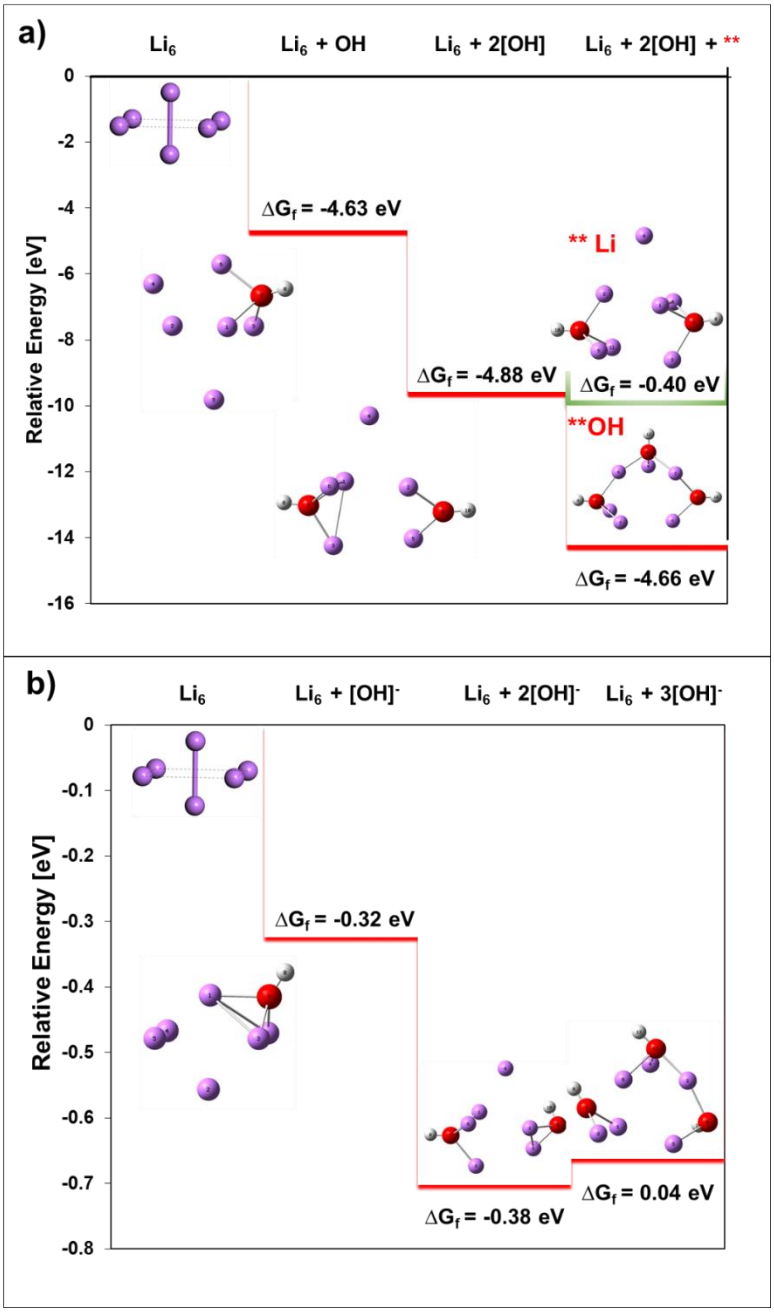

Figure S1. Relative Gibbs Free Energy of Formation for LiOH fragmental growth mechanism. (**a**) Sequential addition of OH while maintaining the total net charge of the cluster equal to zero. (**b**) Every OH added to the cluster includes the addition of 1 electron to the calculation.

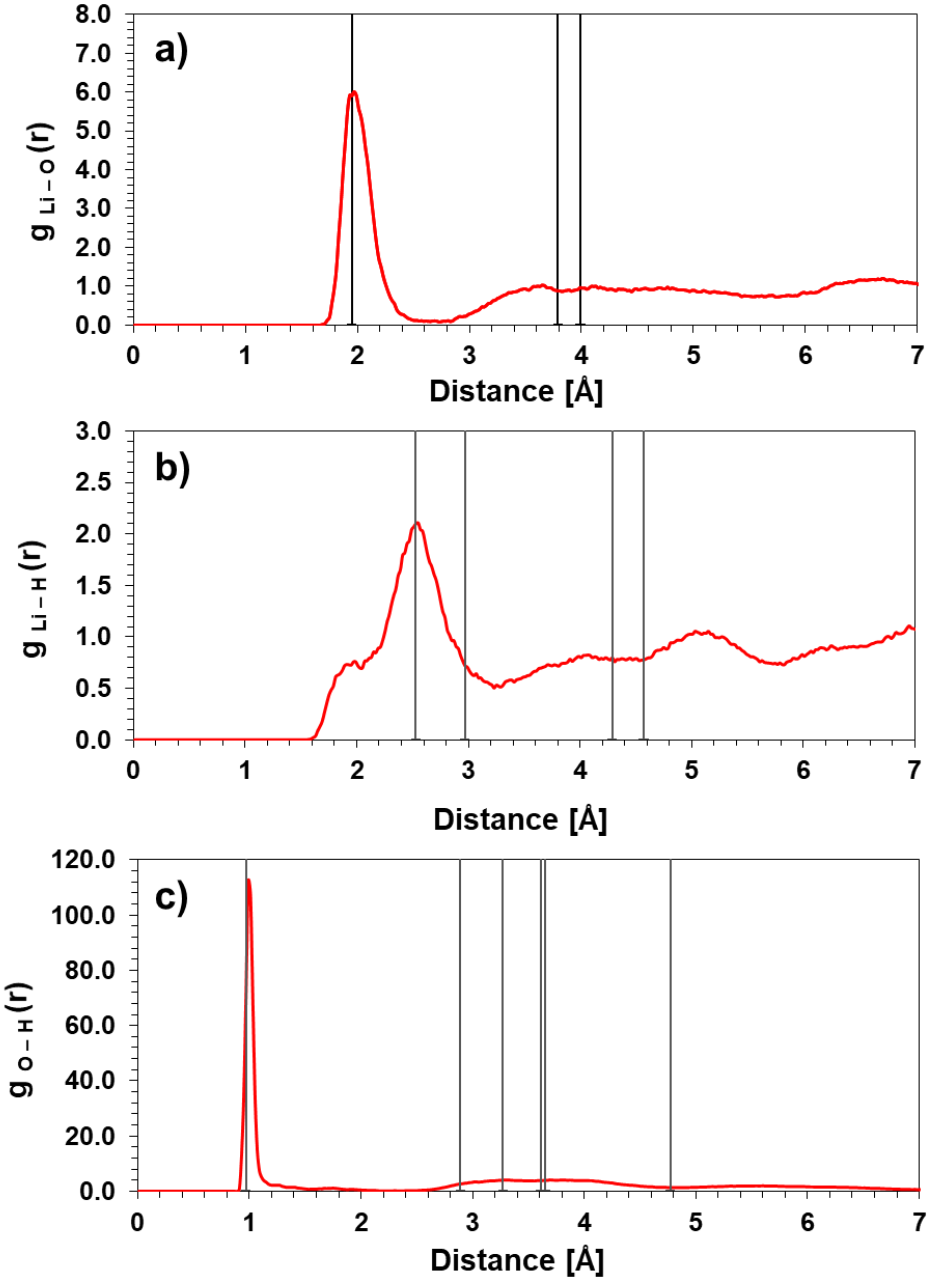

Figure S2. Radial distribution function comparison of crystalline structure of LiOH (black vertical lines) and LiOH AIMD structure after cooling (red curve). (**a**) Distance between Lithium and Oxygen atoms. (**b**) Distance between Lithium and Hydrogen atoms. (**c**) Distance between Oxygen and Hydrogen atoms.

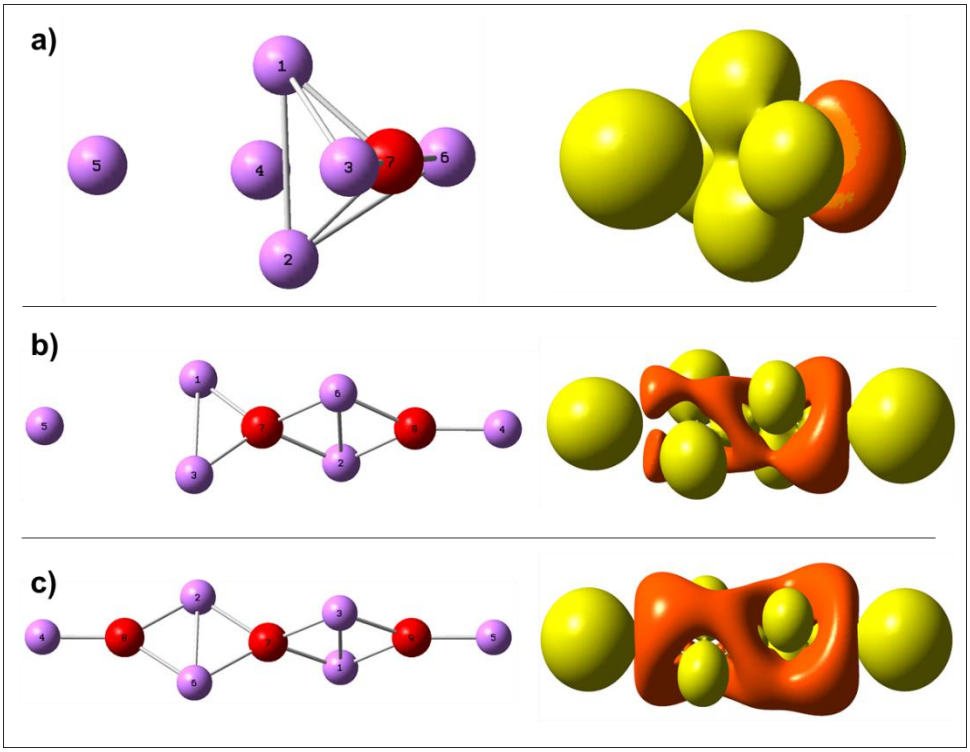

Figure S3. Optimized SEI nanoclusters of Li_2O, structure (left) and corresponding ESP (right). (**a**) Li6 cluster with first addition of Oxygen atom; (**b**) second addition of Oxygen to structure in (a); (**c**) Third addition of Oxygen to structure in (b). Isosurface value of 0.03 a.u. Orange is negative and yellow is positive.

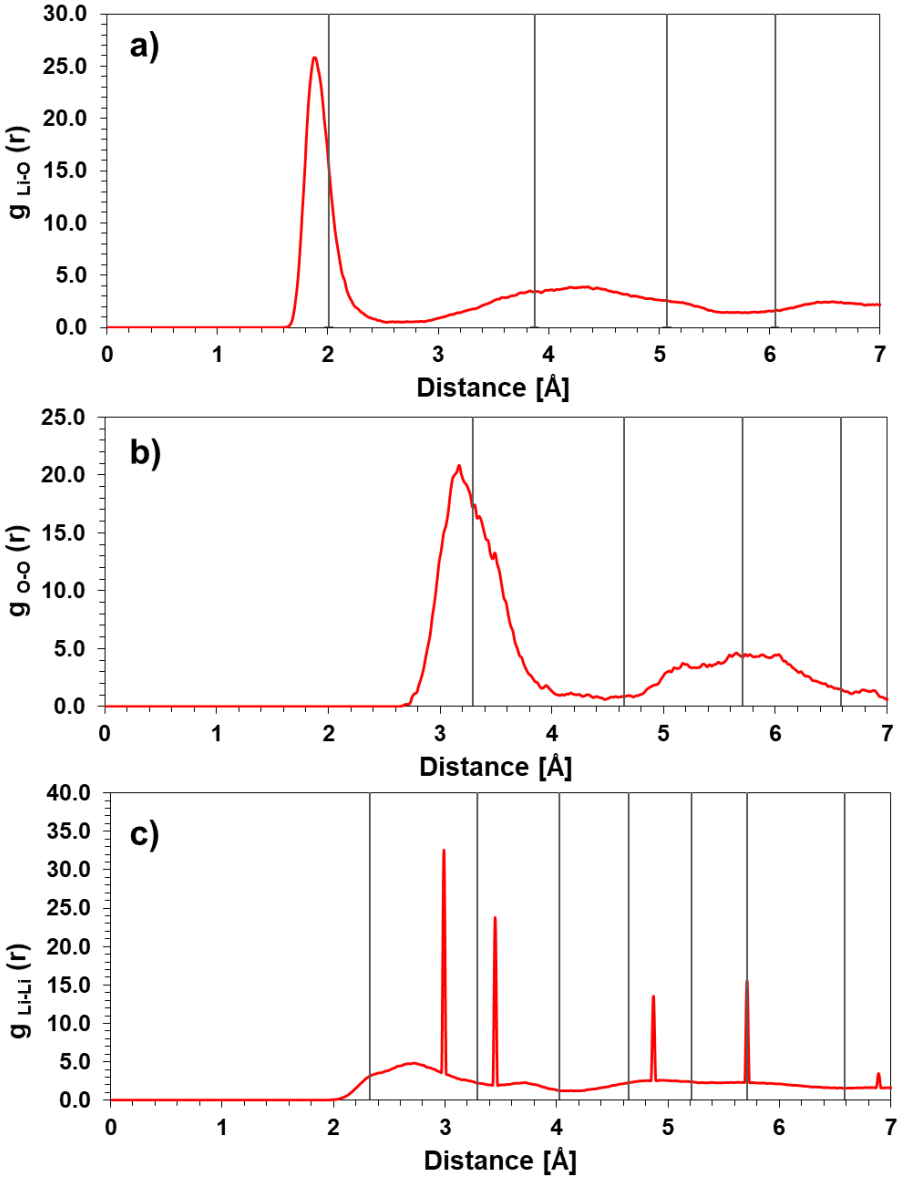

Figure S4. Radial distribution function comparison of Li_2O crystalline structure (black vertical lines) and Li_2O AIMD structure after cooling (red curve). (**a**) Distance between Lithium and Oxygen atoms. (**b**) Distance between Oxygen atoms. (**c**) Distance between Lithium atoms.