energies

Article

First-Principles Study of Amorphous Al_2O_3 ALD Coating in Li-S Battery Electrode Design

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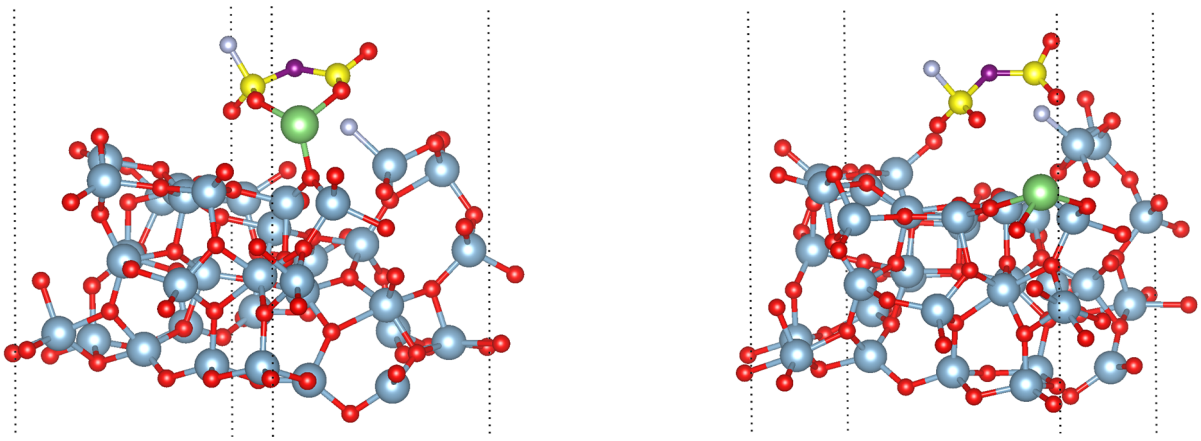

Figure S1. Two lowest energy configurations for LiFSI during adsorption on Al_2O_3 ALD surface. (left) The Li^+ is associated with FSI anion during the adsorption (E_a ~ 2.24 eV), whereas (right) is the optimized geometry where the Li^+ is dissociated from FSI anion during the adsorption (E_a ~ 2.25 eV).

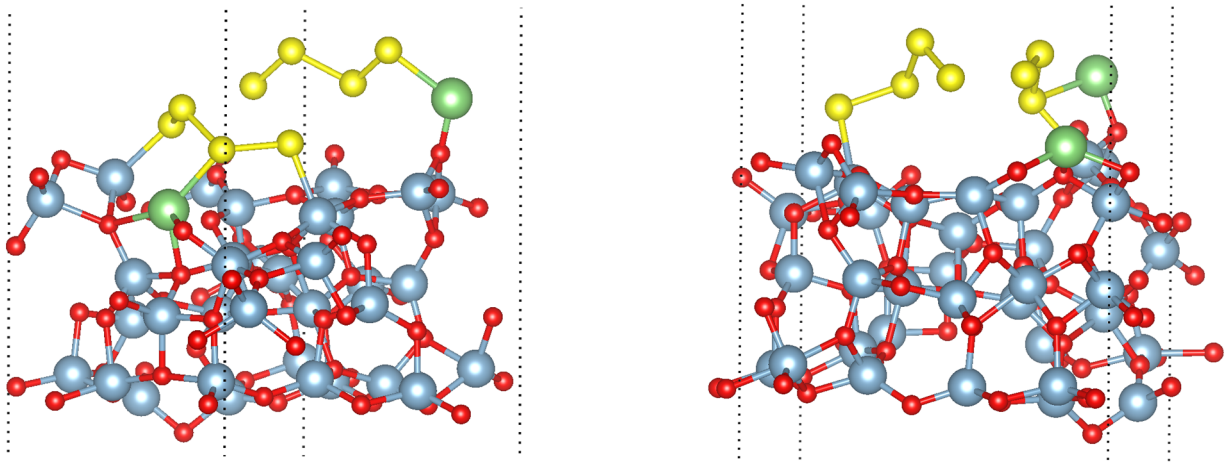

Figure S2. The fragmented Li_2S_8 (with E_a ~ 3.55 eV, left) and Li_2S_7 (with E_a ~ 4.03 eV, right) during the chemisorption on Al_2O_3 ALD surfaces.

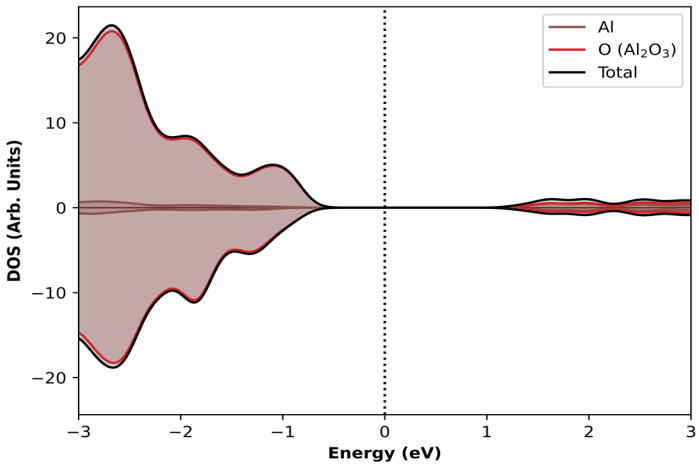

Figure S3. The electronic density of states (DOS) of pristine Al_2O_3 ALD surfaces with band gap ~ 1.60 eV. The black dot line is the Fermi level.