Adsorption study of CO_2 on Li_4SiO_4 nanoparticle via reactive molecular dynamics

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CO_2 emission has been severe environmental issue for several decades due to global warming, and recently lithium silicates have been considered as a promising adsorbent for CO_2 capture. In this study, we investigated CO_2 adsorption mechanism on Li_4SiO_4 at high temperatures (500~650 ℃) using reactive molecular dynamics simulation (i.e. using ReaxFF). First, we developed ReaxFF parameters compatible for bulk and surface systems of Li_4SiO_4, Li_2SiO_3, Li_2CO_3 and optimized the parameters comparing with quantum mechanics (QM) results. With the optimized parameters, we checked phase transition of Li_4SiO_4, Li_2SiO_3 and Li_2CO_3 surface depending on temperature. Second, we observed CO_2 adsorption on Li_4SiO_4 thin layer at different temperatures. In these reactions, we predict thin bilayer and double shell formation on Li_4SiO_4 surface after CO2 adsorption. In addition, multilayer system (Li_4SiO_4-Li_2SiO_3-Li_2CO_3) was modeled to observe the diffusion of Li^+ and O^{2-} ions after thin bilayer formation. The thermal conductivity was estimated by analyzing the temperature profile. Finally, in order to investigate the overall reaction mechanism, we performed time-dependent CO_2 adsorption simulation of Li_4SiO_4 spherical nanoparticle.