DFT Calculation of Molecular Adsorption on Chrysotile Asbestos Surface

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The interaction of small organic molecules with the chrysotile asbestos surface, $Mg_3Si_2O_5(OH)_4$, was investigated by means of density functional theory, to reveal the specific property of molecular adsorptions on the inorganic surface. Chrysotile is composed of tetrahedral SiO_4 and octahedral $MgO_2(OH)_4$ with SiO apical oxygen shared and is cylindrically-curved like carbon nanotubes. We used three kinds of chrysotile models; (i) periodic boundary conditions (PBC) system model, i.e., infinite repeat of $Si_2Mg_3O_5(OH)_4$, (ii) cluster model, i.e., part of PBC model, and (iii) octahedral sheet (O-sheet) model, i.e., infinite repeat of $Mg(OH)_2$. For simplification, we assumed all the structures were flat, which is called lizardite form. The geometry optimization for each model was performed by means of DFT (PBEPBE) with 6-31G(d) basis set. The obtained structural parameters for PBC and cluster models compared well with the experimental data. The layer stacking interaction energies (adhesion energies) were 26.2 and 4.7 kcal/mol per formula unit for PBC and O-sheet models, respectively. The adhesion energy of the PBC model is due to the hydrogen bonding between basal SiO and external MgOH and it is comparable to the energy of 3 hydrogen bonds. We estimated the molecular adsorption energies by using the cluster model and small molecules, such as H_2O, NH_3, CH_3OH, CH_3NH_2 and CH_3COOH. We found that the interaction of those organic molecules with the inorganic surface (with OH group) was equivalent to organic hydrogen bonding: the interaction energy was about 6 kcal/mol for each. It is noteworthy that the electronegative atoms of adsorbing molecules are attractive above OH groups on the surface, while the electropositive atoms of adsorbing molecules are attractive above the cavity which is formed among between positive OH groups. As a result, electropositive as well as electronegative molecules adsorb on chrysotile by electrostatic interaction.

Fig. 1. Crystal Structure

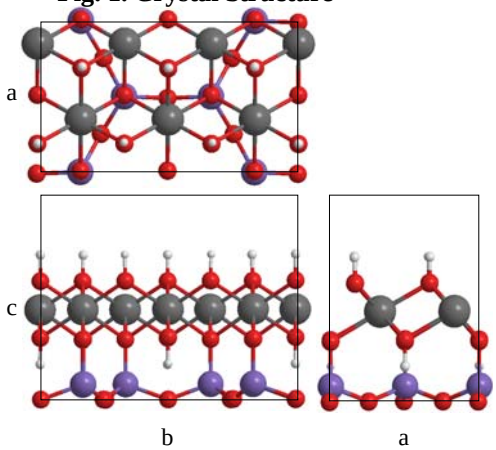
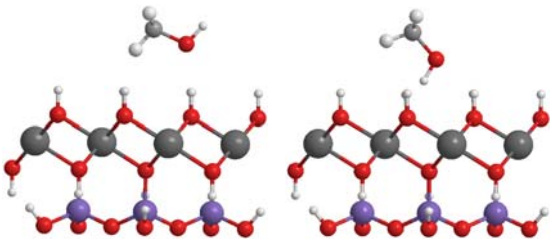


Fig. 2. Molecular Adsorption on Cluster Model



E_{ads} = –5.52 kcal/mol E_{ads} = –7.62 kcal/mol