First-principles study of molecular water adsorption on α-Al_2O_3(0001): Influence of hydrogen isotope

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The reaction of adsorbed molecule water on the α-Al_2O_3(0001) surface is studied by a first-principles molecular dynamics (FPMD) based on density functional theory (DFT). We used both D_2O and T_2O that substituted the hydrogen of the water molecule to examine the effect of the hydrogen isotope. The atoms of the clean alumina surface have been relaxed internally with respect to the atomic positions of the bulk crystal. The oxygen atom of the water molecule adsorbs on the Al atom of the outermost surface layer, the entire molecule water inclines at the direction of a hollow site, and a molecular plane is nearly parallel to the surface. The adsorption is mainly due to the contribution from water lone pairs into unoccupied *p* orbital of aluminium atom of surface Al. The behavior of dissociation and the adsorption of the hydrogen atom of the water molecule is clarified from the FPMD calculation, and it has been understood that the adsorbed site is favorable rather the second neighbor than the nearest-neighbor of the position of surface oxygen.