# Adsorption, dissociation, and dehydrogenation of water monomer and water dimer on the smallest 3D aluminum particle. The O—H dissociation barrier disappears for the dimer.

Autorzy

Jerzy Moc

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Streszczenie

We present a detailed mechanistic study on the interaction and reaction of water monomer and water dimer with the smallest 3D aluminum particle (Al6) by employing density functional and explicitly correlated coupled cluster CCSD(T)-F12 theories. Water adsorption, dissociation, and dehydrogenation are considered. For the monomer reaction, where core–valence correlation and an extrapolation to the complete basis set limit is allowed for, our coupled cluster calculations predict the O–H dissociation barrier of about 2 kcal/mol. For the dimer reaction, two distinct reaction paths are identified, initiated by forming separate dimer complexes wherein (H2O)2 adsorbs mainly via the oxygen atom of the donor H2O molecule. The key O–H dissociation transition states of the dimer reaction involve a concerted migration of two H atoms resulting in the dissociation of the donor molecule and formation of the OH–water complex adsorbed on the metal cluster’s surface. The most remarkable feature of both dimer reaction energy profiles is the lack of the overall energy barrier for the (rate-determining) O–H dissociation. The hydrogen bond acceptor molecule is suggested to have an extra catalytic effect on the O–H dissociation barrier of the hydrogen bond donor molecule by removing this barrier. A similar effect on the dehydrogenation step is indicated.

Adres publiczny

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Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html