

Abstract for a poster for the ES2015 of APS

Adsorption and dissociation of H₂O monomer on ceria(111): Density functional theory calculations

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The adsorption properties of isolated H₂O molecule on stoichiometric and reduced ceria(111) surfaces are theoretically investigated by first-principles calculations and molecular dynamics simulations. We find that the most stable adsorption configurations form two hydrogen bonds between the adsorbate and substrate. The water molecule is very inert on the stoichiometric surface unless up to a high temperature of 600 K. For the reduced surface, we find that the oxygen vacancy enhances the interaction. Moreover, simulations at low temperature 100 K confirm that it is facilitated for water to dissociate into H and OH species.

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