S1-P005

Water-spliting on ultrathin MgO(100) film on Ag(100)

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Water dissociation on oxide surface has been researched in many fields because of its importance as fundamental phenomenas. MgO(001) is a good model system to understand heterogeneous catalysis, gas sensors, ground-water contaminants, and atmosphere chemistry. Over decades, ultrathin film of MgO on Ag(100) have attracted research activities thanks to its enhanced catalytic property. Correlation of the oxide and the metal, potential screening, charge fluctuation from interface reconstruction makes different energetics of hydroxylation of waters on film. We calculate the water-spliting energetics under the vacuum system.

Keywords: MgO, Water, thin film, catalyst, hydroxylation