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【183】DFT Study of Water Adsorption on Ca-Doped (001)-MgO Surfaces

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Combined hydration/dehydration processes of oxide/hydroxide systems - e.g. CaO/Ca(OH)₂ - can be used for storage of industrial excess heat. Exothermal hydration of CaO is fast and complete at ambient temperature; however, dehydration requires high temperatures. A system operable at lower temperatures would be desirable.

A candidate is the system MgO/Mg(OH)₂. However, hydration of the oxide is incomplete at room temperature. Studies of the adsorption behaviour of water on MgO-surfaces suggest kinetic reasons. A previous DFT study found that water does not dissociate at MgO-surfaces, whereas on CaO-surfaces hydroxyls are formed.

In the present work we investigate the effects of Ca-doping of the (001)-MgO-surface on the formation and stability of hydroxyls.

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