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Interfacial reactions of MgO in aqueous environments: Insights from machine learning molecular dynamics

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Interfacial reactions on magnesium oxide (MgO) in aqueous solutions have diverse implications in environmental systems. Iron (Fe) is a common impurity found in naturally occurring MgO which might affect the surface reactions. Here, we investigated the energetics of ion adsorption and surface metal dissolution on the pristine and Fe-doped MgO (001) surfaces in water by using machine learning potentials coupled with metadynamics simulations. The adsorption of a (bi)carbonate ion was achieved by first dehydrating water coordinated with the magnesium (Mg) or Fe site. The (bi)carbonate ion adsorption is thermodynamically favorable on both pristine and Fe-doped surfaces. However, the dissolution of surface Fe had smaller energy barriers and was more favorable than Mg. The propensity of leached Fe^{2+}ions to neutralize the basicity of the hydration layer is likely responsible for the observed low reactivity of Fe-doped MgO, leading to a passivation effect at the interface.

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