Short Communication

The Interactions between High Temperature Water and Fe₃O₄(111) by First-Principles Molecular Dynamics Simulation

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The interactions between high temperature water and oxide film Fe₃O₄(111) are investigated using a Born-Oppenheimer molecular dynamics simulation within the framework of density functional theory. A periodic twelve-layer slab covered with 21 water molecules is employed to simulate the interfacial reaction behavior. It can be observed in the simulation that the spontaneous dissociation processes of H₂O molecules occur on the Fe₃O₄(111) surfaces and the partial density of states demonstrates the hybridization bonding between 2p orbital of O atom and 3d orbital of Fe atom. There is an obvious charge transfer between the oxide film/electrolyte interface, whereas the charge transfer of the middle layers of substrate and solution is not significant.

Keywords: Magnetite; High temperature water; First principles molecular dynamics; Interfacial reaction

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