Structure and reactivity of Iron Oxide Nanoparticles

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The design of nanoscale materials for creative and sustainable engineering applications is predicated on an accurate description of the structure, properties, and reactivity of these materials. As an example, iron oxide nanoparticles are widely used for a range of biomedical, chemical, and environmental engineering applications, such as directing drug delivery in the body or controlling the mobility of toxic metals in water, but the physical and chemical factors governing their reactivity have only slowly begun to emerge with the aid of ab initio calculations and molecular modeling. We have designed a new gas-phase iron oxide/silica nanoparticle capable of catalyzing carbon nanotube growth on the surface with high yield and selectivity, and present the mechanism for acetylene decomposition and carbon ring formation on this catalyst, as computed using spin-unrestricted density functional theory calculations and Car-Parrinello molecular dynamics simulations. We also present the structure and energetics of various surface terminations of clean and hydrated magnetite Fe3O4 (110). These systems and others demonstrate the feasibility of using ab initio calculations as a basis for studies bridging length and time scales between model systems and real systems probed in experiments.