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ReaxFF-based molecular dynamics studies on reactions at complex material surfaces

ADRI VAN DUIN, Penn State

The ReaxFF method provides a highly transferable simulation method for atomistic scale simulations on chemical reactions at the nanosecond and nanometer scale. It combines concepts of bond-order based potentials with a polarizable charge distribution. Since it initial development for hydrocarbons in 2001, we have found this concept to be highly transferable, leading to applications to elements all across the periodic table, including all first row elements, metals, ceramics and ionic materials. In this presentation we will provide an overview of recent developments of the ReaxFF method for reactions at the complex material interfaces, in particular TiO_2/water, silica/water and graphite/oxygen interfaces. We will describe the ReaxFF parameter development process and show how, by employing parallel molecular dynamics methods, ReaxFF can assist in bridging the gap between atomistic-scale simulations and experiment. We will also discuss new developments in metadynamics and Monte Carlo based implementations of ReaxFF, which enable us to extend molecular dynamics simulation times to beyond hundreds of nanoseconds.