

Applications of the ReaxFF force field to complex materials and interfaces

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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 its initial development for hydrocarbons in 2001, we have found that this concept is transferable to applications to elements all across the periodic table, including all first row elements, metals, ceramics and ionic materials. For all these elements and associated materials we have demonstrated that ReaxFF can accurately reproduce quantum mechanics-based structures, reaction energies and reaction barriers, enabling the method to predict reaction kinetics in complicated, multi-material environments at a relatively modest computational expense.

This presentation will describe the current concepts of the ReaxFF method, the current status of the various ReaxFF codes, including parallel implementations. Also, we will present an overview of recent applications to a range of materials of increasing complexity, with applications to combustion, catalysis, aqueous phase chemistry and material failure.