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The ReaxFF method - new applications and developments

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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 it 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 reproduce quantum mechanics-based structures, reaction energies and reaction barriers with reasonable accuracy, 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 and recently developed hybrid Grand Canonical Monte Carlo options - which significantly increase its application areas. Also, we will present and overview of recent applications to a range of materials of increasing complexity, with a focus on applications to combustion, biomaterials, batteries, tribology and catalysis.