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Reactive force fields – current status, needs, and challenges

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ABSTRACT

Simulation-based predictive design of materials is a vital strategy towards fulfilling the directive posed by the National Materials Genome Initiative. The key ingredient in classical atomistic simulations is the interaction potential, or force field, which describes the energetic interplay between atomic constituents. Effective simulation-based materials design requires great flexibility in choosing the chemical composition of the material under development. It furthermore entails the ability to generate realistic atomistic structures of bulk materials, defects, and interfaces, in order to predict materials properties and behaviors accurately. Hence, the requirements for force fields used in atomistic simulations are: (1) computational efficiency, (2) adaptability, (3) transferability, and (4) accuracy. As to (1), to generate realistic structures containing extensive features and defects, simulations must include large numbers of atoms and be carried out over extensive periods of time. The more efficiently atomic interactions can be described and computed, the larger can simulate structures and the more detail can be accounted for in the temporal evolution of these structures. Indeed, in some cases structural developments include chemical reactions and phase transformations, which connotes requirement (2), i.e., force fields must be able to account for changes in bonding character, charge transfer, and coordination number change. Requirement (3) refers to ability of force fields to accommodate a wide variety of chemical species, the ensuing bonding types, and local structural symmetries. Finally, requirement (4) indicates that force fields not only need to accurately predict nearest-neighbor distances and bonding energies, but also properties that depend on higher order derivatives, e.g., vibrational properties, thermal expansion coefficients, etc. All these requirements call for the ability to develop force fields describing the interactions between exponentially expanding numbers of species combinations. The computational framework to accommodate this demand of force field features and parameterizations is currently sorely lacking. This presentation provides a summary of the current state-of-the-art, as well as examples of successes and shortcomings, and is intended to spur a dialogue concerning these demands and challenges.