Atomistic-scale simulations of realistic, complex, reactive materials: overview of the ReaxFF/e-ReaxFF reactive force fields and their applications to 2D materials

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Abstract:

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[1], 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[2]. 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. At this moment, over 1000 publications including ReaxFF development of applications have appeared in open literature and the ReaxFF code – as implemented in LAMMPS, ADF, or in standalone-format – has been distributed around the world.

This presentation will describe the current concepts of the ReaxFF method, the current status of the various ReaxFF codes, including parallel implementations and acceleration methods. Also, we will present and overview of recent and past applications to complex materials, with a focus on 2D-material defect chemistry[3-4], metal deposition[5-6] and recent developments for expansion of ReaxFF for events in graphitic materials that require explicit electrons (e-ReaxFF)[7].

References

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