Development and applications of the ReaxFF reactive force field method and its incorporation in a multiscale modeling framework (CMDF)

Adri van Duin*, Markus Buehler and William Goddard
California Institute of Technology
* duin@wag.caltech.edu

ReaxFF is a bond-order dependent force field method that includes a geometry-dependent polarizable charge distribution and enables reactive, atomistic scale dynamic simulations at a computational expense magnitudes lower than quantum mechanical (QM) simulations.
While initially developed for first-row elements, over the last years we found the method to be highly transferable, allowing us to develop ReaxFF descriptions for covalent, metallic, ionic and mixed systems all across the periodic system (e.g. [1-4]. This presentation will discuss the background of the ReaxFF methodology and will show highlights of its past and ongoing applications, which include fuel cell chemistry, high-energy materials, carbon nanotube growth and semiconductor materials.
We believe that ReaxFF provides a critical methodology for multiscale simulations on reactive systems. On one hand, ReaxFF paramerization is largely dependent on QM-data, describing the geometry and relative energy of relevant systems including transition states. As such, ReaxFF provides a tool to perform QM-informed molecular dynamics on large (>>1000 atoms) atomistic systems. Furthermore, the high transferability of ReaxFF makes the method highly suitable as a 'glue' between less transferable, but even less expensive non-reactive force field methods. To exploit the ReaxFF capabilities in multiscale simulations we have incorporated this methodology in the CMDF-framework, which is a Python-based interface between different computational engines and have recently applied the CMDF framework to crack propagation in silicon [5]. This presentation will discuss recent ReaxFF-related applications within the CMDF framework.

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