The computational materials design facility (CMDF): A new framework for multi-scale multi-paradigm modeling

Markus J. Buehler, Jef Dodson, William A. Goddard

Materials and Process Simulation Center
California Institute of Technology, Pasadena, CA

It has always been the dream of scientists to predict the properties of new materials by theoretical modeling or computer simulation from a very fundamental, *ab initio* perspective. Since all properties of all materials are in principle describable by quantum mechanics (QM), one could, in principle, replace current empirical methods used to model materials properties by first principles or *de novo* computational design of materials and devices. Why has this not happened yet? The reason is that there are several major problems. For instance, direct *de novo* applications of QM are practical for systems with \( \sim 10^2 \) atoms whereas the materials designer deals with much larger systems of \( \sim 10^{22} \) atoms. The solution to filling this enormous gap is to factor the problem into several overlapping scales each of which can provide a scale factor of \( \sim 10^4 \). This objective is achieved by the development of seamless coupling methodologies between different modeling paradigms across the time and length scales. This scheme allows accurate predictions of the properties for novel materials never previously synthesized and permits estimates of the intrinsic bounds on properties avoiding wasting time on impossible challenges.

We therefore focus on the development and application of new computational methods for modeling of complex phenomena that require multi-scale and multi-physics treatment involving proper handling of chemistry that is critical in particular for modeling biological systems (the “Computational Materials Design Facility”). These methods play a critical role in research endeavors in the field of modeling phenomena, in particular to describe biological processes and nanomaterials. The method couples quantum mechanical (QM) methods (e.g. DFT theory), the first principles reaxFF reactive force field, empirical all atom force fields (FF, e.g. DREIDING, AMBER, and CHARMM), multi-body potentials (e.g. EAM for metals, TERSOFF for carbon and silicon), as well as continuum methods (e.g. the APBS (Poisson-Boltzmann based) FE method to model implicit solvants, and FE methods to model elasticity and plasticity). It also includes new methods to speed up calculations such as the parallel replica method. Coupling of different methods is achieved based on a modern Python scripting environment to allow seamless combination of different monolithic simulation codes in an object-oriented style to allow straightforward information exchange between different codes. This is further facilitated by our newly developed global data structure that contains generic information about the system studied.

We report application of our new methods in hybrid models incorporating reactive and nonreactive force fields. Among other problems, we present modeling of crack propagation in silicon and oxidation of an aluminum surface.