WebFF: A Smart Force-Field Repository for Polymers and Soft Materials[*]

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Abstract

The vision of the Materials Genome Initiative (MGI)[1,2] is a new R&D paradigm enabling accelerated materials design via computation leading to a shortening of the time and cost needed to bring new materials to market. This new paradigm will be fostered through the creation of national infrastructure for materials data sharing and analysis that supports integrated multiscale modeling of materials[3] from the quantum or molecular level, upward in both length and time scale to the continuum scale represented by structural components. The NIST role in the MGI is to create the infrastructure for the effort through the development of 1) standards and tools for the representation and interoperability of materials data, and 2) techniques and standards for the interoperation of modeling systems at multiple length and time scales.

In a hierarchical approach to materials modeling, molecular dynamics (MD) calculations are integral to calculating properties and phenomena at length scales ranging from Angstroms to tens of nanometers, on time scales up to tens of microseconds. In addition, these models provide the foundational level upon which progressive, multi-scale models are built. A critical data need required to support MD simulations for materials research are widely available, highly accurate, and validated force field data. In this talk, we will describe WebFF, an open and extensible, smart force field repository based on Amber and CFF type molecular potentials designed to support the MGI for polymers and closely related soft materials. The repository consists of three main components: 1) a web-client interface enabling wide and open access; 2) a software engine to provide robust workflow functionality; and 3) an extensible, multi-table database for the purpose of encouraging and supporting validated data sharing. The repository functions in two main modes of access. The workflow mode supports input of chemical structures, automated force field assignment, and output to support MD calculations. The data sharing mode supports input of new force-field data to the extensible database model to support validated data sharing. The seminar will demonstrate the workflow mode as a means of facilitating the use of accurate force-field data in MD simulations for a number of open source simulation engines. The methods, requirements and goals of force field data sharing for the repository will also be described.

References

1. “Materials Genome Initiative for Global Competitiveness,” Office of Science and Technology Policy, Executive Office of the President, Washington, DC, (2012).

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2. James A. Warren, Boisvert, Ronald F., “Building the Materials Innovation Infrastructure: Data and Standards,” NISTIR 7898, National Institute of Standards and Technology, Gaithersburg, MD, (November 2012).
3. “Integrated Computational Materials Engineering,” National Research Council, The National Academies Press, Washington, DC, (2008).