

Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Analytic bond-order potentials: from the electronic structure to million atom simulations

Drautz, Ralf, ralf.drautz@rub.de, Ruhr-Universität Bochum

ABSTRACT

The analytic bond-order potentials (BOPs) are derived by systematically coarse graining the electronic structure from density functional theory into effective interatomic interactions. This derivation comprises expressions for charge transfer and magnetism, including noncollinear magnetism, that are obtained directly from density functional theory, so that the BOPs constitute a coherent simplified description for modeling bond making and breaking in covalent and metallic materials. Similar to the structure and functional form of the BOPs, their parameterization may also be obtained by projection from density functional theory. In this discussion, I will outline the structure and derivation of the BOPs and summarize their parameterization. I will discuss applications of the BOPs in simulations of refractory elements, iron and iron carbon. The relation of the BOPs to other methods such as recursion, the Kernel Polynomial Method, or the Fermi Operator Expansion will be briefly reviewed and the integration of the BOPs into established codes for simulations with millions of atoms will be highlighted.