

Toward universal embedded-atom method – empirically adjusted and consistent set of atomic densities for all elements of the periodic table

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The Hartree-Fock-Slater model of atom has been modified by using individual values of the exchange parameter, α_{ex} , for each atom. Each value of α_{ex} was adjusted to reproduce the empirical value of the first ionization energy of the atom considered. The expectation values of energies and radial functions for all elements of the periodic table have been evaluated on the basis of the Hartree-Fock-Slater model and individual exchange parameters. Qualitatively, the expectation values compare well with Mann's numerical Hartree-Fock values but contain some influence of correlation and relativistic phenomena. A consistent set of universal atomic electron density tables for all elements of the periodic table, suitable for embedded-atom method (EAM) type calculations, is presented. We considered the electron density distribution as the key variable linking the total energy and interparticle separation in EAM molecular dynamics study. The universal set of atomic densities have been tested using XMD molecular dynamics package.

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