Semi-infinite metal: thermodynamic characteristics and effective pair interionic potentials

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Theoretical studies of equilibrium properties of a metal surface is very difficult, because an electronic subsystem of bounded metal is very spatially nonuniform. It essentially complicates the consecutive account of many-particle effects in an electronic subsystem. The greatest successes in studying of electronic properties of a metal surface have been attained within density functional theory (DFT). However the study of properties of a metal surface which are caused by discreteness of the ionic subsystem is problematic, as method of constructing necessary energy functionals is not known.

In presented work systematic perturbation theory for bounded metals, described by nonlocal pseudo-potentials, is developed. The semi-infinite jellium [1,2] is used as the reference system and the perturbation theory with respect to the "difference potential" (that is the difference between the pseudo-potential of ions and the electrostatic potential of the semi-infinite jellium positive background) is constructed.

Potentials of the interionic interaction has been great interest both for this theory and for atomistic modeling of materials [3]. We investigate potential of pair interionic interaction in the semibounded metal with use of different local field corrections.

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