RESEOS – equation of state based on the 'confined atom' model

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The main problems in the description of energy spectrum of electrons by using self-consistent field models are concerned with the account of intermediate states between bound states localized in the atomic cell and free states that can be described by using quasi-classical approximation. In the INFERNO model [1] resonances of density of states in the continuum play an important role for the description of such states. Resonances are connected with quasi-stationary states and appear under the pressing-out bound states to continuum with the growth of density of matter [2,3]. In the region of the electron transition from discrete spectrum to continuum the contribution of resonance to the electron density is similar to the contribution of corresponding bound level. It results in a smooth behavior of thermodynamic functions under the pressure ionization [4,5].

The algorithm for the computation of self-consistent atomic potential taking into account resonances is developed. Calculations of aluminium and uranium equations of state are performed in a wide range of temperatures and densities. The obtained results are compared with the Hartree-Fock-Slater model including energy bands (the so-called quasizone model) and with experimental data.

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