

# **AB INITIO MODELING OF METALS WITH HOT ELECTRON SUBSYSTEM**

V.V. Stegailov

*Joint Institute for High Temperatures RAS  
Moscow Institute of Physics and Technology (State University)*

The description of the electron-ion relaxation in condensed phase of real substances with excited electrons is currently an actual theoretical problem that has no general methods of solution in the framework of quantum molecular dynamics. As a tool of analysis of the electron-phonon interaction in solid phase the finite-temperature density functional theory is applied. The phonon dispersion and the electron DOS studies are carried out for the two-temperature system “cold lattice – hot electrons”. The analysis was performed of the influence of electron temperature on stability of simple and d-metals (Al, Au and Ni). The results point to the substantial redistribution of electron densities and change of the interionic interaction at electron temperatures above 2-3 eV.