Quantum mechanical calculations in computational materials science

Alexey Yanilkin VNIIA

The presentation will consider the use of quantum mechanical calculations on supercomputers for various material science problems. As such problems, investigation of the thermoelectric properties of materials, the construction of phase diagrams, diffusion properties, and the development of classical interatomic interaction potentials are considered. The main computational requirements for such calculations are discussed, as well as the use of the VNIIA supercomputer.