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Uranium phase diagram from first principles ALEXEY YANILKIN, IVAN KRUGLOV, KIRILL MIGDAL, ARTEM OGANOV, PAVEL POKATASHKIN, OLEG SERGEEV, Dukhov Research Institute of Automatics (VNIIA), 127055, Russia, Moscow, Suschevskaya st., 22. — The work is devoted to the investigation of uranium phase diagram up to pressure of 1 TPa and temperature of 15 kK based on density functional theory. First of all the comparison of pseudopotential and full potential calculations is carried out for different uranium phases. In the second step, phase diagram at zero temperature is investigated by means of program USPEX and pseudopotential calculations. Stable and metastable structures with close energies are selected. In order to obtain phase diagram at finite temperatures the preliminary selection of stable phases is made by free energy calculation based on small displacement method. For remaining candidates the accurate values of free energy are obtained by means of thermodynamic integration method (TIM). For this purpose quantum molecular dynamics are carried out at different volumes and temperatures. Interatomic potentials based machine learning are developed in order to consider large systems and long times for TIM. The potentials reproduce the free energy with the accuracy 1-5 meV/atom, which is sufficient for prediction of phase transitions. The equilibrium curves of different phases are obtained based on free energies. Melting curve is calculated by modified Z-method with developed potential.

Vasily Zhakhovsky
Florida State University

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