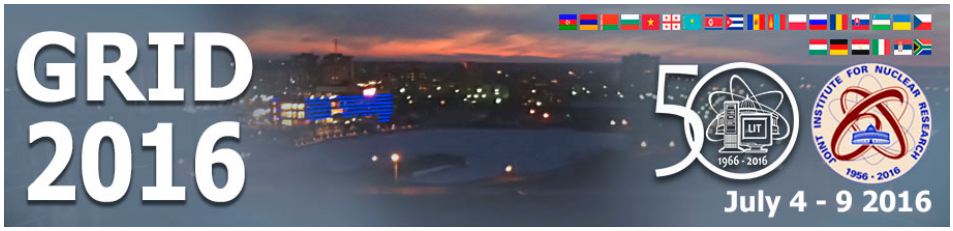

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PARAMETRIZATION OF THE REACTIVE MD FORCE FIELD FOR Zn-O-H SYSTEMS

Monday, 4 July 2016 17:30 (1 hour)

In this contribution we describe a procedure of optimizing the molecular dynamic force field for Zn-O-H chemical systems by means of a new parallel algorithm of a multifactorial search for the global minimum. This algorithm allows one to obtain numerous parameters of the ReaxFF classical force field based on quantum chemical computations of various characteristics of simple compounds. The force field may be then used for simulating of large-scale chemical systems consisting of the same elements by means of classical molecular dynamics. Our current implementation of the algorithm is done in C++ using MPI.
We compare characteristics of simple compounds, obtained by 1) quantum chemical techniques, 2) molecular-dynamic methods using reference parameters of the force field, and 3) MD methods using optimized parameters of the force field. With the optimized parameter set we perform MD simulations (using LAMMPS package) of crystals of zinc and zinc oxide of various modifications at the room temperature.
Finally, we compare results of the parameter optimization procedure by means of the algorithm described above and results of a parallel implementation of an evolutionary approach to minimum search using dynamic models of Zn and ZnO crystals. Also we discuss advantages and disadvantages of the both methods and their efficiency for extremal problems.
All computations are performed with machines of the distributed scientific complex of the Faculty of Physics of St Petersburg State University.

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