

Application of atomistic simulation for modeling of gas hydrates

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The continuing rapid development of theoretical and computational methods of atomistic simulations during past decades provides a basis of analysis and prediction tools for chemistry, material science, condensed matter physics, molecular biology and nanotechnology. Nowadays molecular dynamics (MD) method that describes motion of individual atoms by the Newton's equations is a research tool of highest importance. The computational speed and the efficiency of parallelization are the main factors that pose limitations on the length and time scales accessible for MD models (the achievable extremes for classical MD are trillions of atoms and milliseconds, a typical MD step being 1 fs).

We can distinguish critical avenues in the development of high performance MD models. Quantum MD models demonstrate much higher requirements to the data communication speed and hence to the interconnect properties. The deployment of hybrid architectures for electronic structure calculations and quantum MD is not mature enough. Classical MD models are less demanding with respect to data communication. The main limitation in classical MD is the computational complexity of interatomic potentials that is determined by the performance of supercomputer nodes. Therefore hybrid architectures of nodes are considered as a major perspective. In this work we compare different hardware for the software packages widely used for atomistic modeling.

We use molecular dynamics to study properties of methane and hydrogen hydrates. Gas hydrates are crystalline water-based inclusion compounds in which guest molecules are trapped inside cavities of the hydrogen-bonded water network. Several clathrates and filled-ice structures are known. Structure type primarily depends on guest size, temperature and pressure. Gas hydrates allow compact storage of hydrocarbons since one volume of hydrate may contain 180 volumes of gas. Recently, they have attracted interest due to the possibility of being used for hydrogen storage. The pure hydrogen hydrates form at very high pressure, however, the addition of a promoter molecule, for example, tetrahydrofuran or methane, significantly reduce the formation pressure. Practical usage of hydrogen hydrates requires knowledge of their thermodynamic and kinetic properties, mechanisms of formation and decay in a wide range of pressures and temperatures.

In this work, we perform coexistence simulations of methane hydrates for pressures up to 5000 bar for different water models. We calculate the kinetic stability boundary of the superheated metastable sI structure and analyze the effects of the heating rate, system size and cage occupancy [1]. We also report molecular dynamics simulation of several possible structures for the new hydrogen hydrate clathrate. We show the strength of molecular simulation as a supplement tool for the analysis of experimental data [2].

References:

- [1] Smirnov G.S., Stegailov V.V. J. Chem. Phys. 136, 044523 (2012).
- [2] Smirnov G.S., Stegailov V.V. J. Phys. Chem. Lett. 4, 3560 (2013).