

Abstract Submitted
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Atomistic level description of phase diagram of gas clathrate hydrates with complex gas compositions¹ R. BELOSLUDOV, H. MIZUSEKI, IMR, Tohoku University, Y. KAWAZOE, NIHC, Tohoku University, O. SUBBOTIN, V. BELOSLUDOV, Nikolaev Institute of Inorganic Chemistry, SB RAS — An approach has been realized that allows us to construct a p-T phase diagrams of various gas hydrates, three-dimensional hydrogen-bonded water structures in which water molecules arrange themselves in a cage-like (host) structure around gas (guest) molecules, with complex gas compositions [1-2]. In order to evaluate the parameters of weak interactions, a TDDFT formalism and LDA technique entirely in real space have been implemented for calculations of vdW dispersion coefficients for atoms within the all-electron mixed-basis approach. The combination of both methods enables one to calculate thermodynamic properties of clathrate hydrates without resorting to any empirical parameter fittings. Using the proposed method it is possible not only confirm the existing experimental data but also predict the unknown region of thermodynamic stability of clathrate hydrates, and also propose the gas storage ability as well as the gas composition for which high-stability region of clathrate hydrates can be achieved. The proposed method is quite general and can be applied to the various non-stoichiometric inclusion compounds with weak guest-host interactions.

[1] R. V. Belosludov et al. J. Chem Phys. 131 (2009) 244510

[2] R. V. Belosludov et al. Mol. Simul. 38 (2012) 773.

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