Description of thermodynamic properties of gas hydrates using interaction potentials evaluated from TOMBO program

R. V. Belosludov[1], O. S. Subbotin[2], H. Mizuseki[3], V. R. Belosludov[2,4] and Y. Kawazoe[4,5]

[1]*Institute for Materials Research, Sendai, Japan*
[2]*Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia*
[3]*Center for Computational Science,KIST, Seoul, Korea*
[4]*Kutateladze Institute of Thermophysics, SB RAS, Novosibirsk, Russia*
[5]*New Industry Hatchery Center, Tohoku University, Sendai, Japan*

In order to construct a *p-T* phase diagrams of various gas hydrates with complex gas compositions, we have developed an original method has been realized [1-3]. The parameters of weak interactions have been evaluated using a time-dependent density-functional formalism and local density technique entirely in real space implemented within the all-electron mixed-basis approach [4]. 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. From this point of view, the present methodology can support experimental explorations of the novel storage materials.

REFERENCES

[1] V. R. Belosludov *et al. Mater. Trans.* **48** (2007) 704.
[2] R. V. Belosludov *et al. J. Chem Phys.* **131** (2009) 244510.
[3] R. V. Belosludov *et al. Mol. Simul.* **38** (2012) 773.
[4] R. V. Belosludov *et al.* in *Handbook of Sustainable Engineering*, ed. by K-M. Lee and J. Kauffman, Springer, New York, (2013) pp. 1215-1247.