Theoretical aspects in realization of functional nanomaterials for energy and medical applications

Rodion Belosludov*

Institute for Materials Research, Tohoku University, Sendai, JAPAN

In order to design materials with novel composition and desirable characteristics it is important to have a good understanding of the atomic-scale chemical and physical properties of materials. Computer simulation has become an indispensable research tool because often experiments require theoretical interpretation and computing power has grown rapidly in the last decade. *Ab initio* methods can potentially offer an independent model of material properties. Moreover, simulation methods, which are based on *ab initio* parametrization of interaction potentials, can be used to perform large-scale simulations at non-zero temperatures. Therefore, we try to accurately estimate the important properties of various materials in order to accelerate the realization of novel materials, hand-in-hand with experiment and propose these materials for energy and medical applications. Here, the recent achievements of our group have been reviewed. Thus, we studied the structural morphology of the core as well as the inorganic/organic interface at the atomistic level in an effort to improve upon the materials currently used in cancer diagnosis [1]. Recently, we have presented a conceptual design for functional 3D porphyrin-based nanostructures, which would bridge the gap between the well-known fullerenes and nanotubes and a new class of the functional nanomaterials, which may potentially be used as analogues of quantum dots for solar cells and imaging/ bioimaging applications [2]. In collaboration with experimentalists, we have shown that the concept using a designable regular MOF material could be applicable to a highly stable, selective adsorption system [3]. We proposed the theoretical model for calculating the thermodynamic properties of nano-porous materials with weak guest-host interactions. In combination with *ab initio* parametrization of interaction potentials, this method enables to calculate thermodynamic properties of nano-porous materials without resorting to any empirical parameter fittings [4].

REFERENCES

1. A. Kasuya et al., *Nature Materials* **3**, 99-102, 2004.
2. R. V. Belosludov *et al. Phys. Chem. Chem. Phys.* **18** (2016) 13503.
3. R. Matsuda *et al. Nature* **436** 238 (2005); H. Sato *et al. Science* **343** (2014) 167.
4. R. V. Belosludov *et al. J. Chem. Phys.* **131** (2009) 244510; R. V. Belosludov *et al. Mol. Simul.* **38** (2012) 773; R. V. Belosludov *et al. J. Phys. Chem. C* **118** (2014) 2587.