First-Principles Modeling of Nanomaterials for Energy Storage Applications

Joongoo Kang[1], Su-Huai Wei[1], and Yong-Hyun Kim[2]

[1]National Renewable Energy Laboratory, Golden, Colorado 80401, USA

[2]Graduate School of Nanoscience and Technology (WCU), Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea

Renewable energy sources like solar and wind are inherently intermittent on a daily and yearly scale. To meet future energy needs, it is thus imperative to develop efficient energy storage materials. As the characteristic length of energy storage materials decreases to nanometer scale, energy storage mechanisms becomes different from those of macroscopic counterparts. Here, we developed first-principles thermodynamic approaches combined with the multiple-histogram method [1] and grand-canonical Monte Carlo simulations to calculate key physical quantities of nano storage systems: (i) heat capacity of nano-materials for thermal energy storage [2], (ii) H_2 adsorption/desorption isotherms of nanoporous materials for hysteretic hydrogen storage [3] and (iii) electrochemical capacitance of nanostructured pseudo-capacitors [4]. The simulated results will be compared with experimental data, and microscopic energy storage mechanisms will be discussed.

This research was funded by U.S. DOE/OS/BES, DOE/EERE and NREL LDRD programs under Contract No. DE-AC36-08GO28308.

[1] P. Chandrachud, K. Joshi, and D. G. Kanhere, *Phys. Rev. B* **76**, 235423 (2007).

[2] J. Kang and Y.-H. Kim, *ACS Nano* **4**, 1092 (2010).

[3] J. Kang, S.-H. Wei, and Y.-H. Kim, *J. Am. Chem. Soc.* **132**, 1510 (2010).

[4] J. Kang, S.-H. Wei, K. Zhu, and Y.-H. Kim, submitted.