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Energy Storage in Nanostructured Materials

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Renewably produced energy by solar and wind technologies should be stored properly for practical use because of their intermittent generation of electricity. The energy can be stored in materials in forms of chemical, electrical, or thermal energies. The current energy-storage materials technologies, however, suffer from their inevitable low energy densities, compared to liquid fuels such as gasoline and ethanol, and thus end up to high cost due to material limitation. In order to overcome the fundamental limit, many scientists and researchers have studied nanostructured materials with more surface areas, tunable storage mechanisms, and better kinetic processes. Because electronic and mechanical properties of nanostructured materials are simply not a miniature of their bulk counterparts, a careful material design is required based on microscopic understanding of the energy storing process. In this talk, I will discuss our recent theoretical efforts and development to understand energy storage mechanisms in nanostructured materials for hydrogen, battery, and electrochemical capacitor applications. We have pioneered dihydrogen adsorption in nanostructured materials with the Kubas coordination [1-3] and lately developed efficient van der Waals potentials within the density functional theory approach [4]. Also very recently we have unraveled reversible lithium intercalation mechanisms in MoO_3 nanoparticles for Li-ion battery electrodes [5], and been developing a microscopic theory of electrochemical and capacitive energy storage.

[1] Y. Zhao et al., Phys. Rev. Lett. **94**, 155504 (2005)
[2] Y.-H. Kim et al., Phys. Rev. Lett. **96**, 016102 (2006)
[3] Y. Y. Sun, Y.-H. Kim, and S. B. Zhang, J. Am. Chem. Soc. **129**, 12606 (2007)
[4] Y. Y. Sun, Y.-H. Kim, K. Lee, and S. B. Zhang, J. Chem. Phys. **129**, 154102 (2008)
[5] S.-H. Lee et al., Adv. Mater. **20**, 3627 (2008)