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Title: Gas Adsorption and Renewable Energy Application: Lesson from Quantum Mechanics

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Renewable energy applications need a proper control of three important gases, i.e., hydrogen (H2), oxygen (O2), and carbon dioxide (CO2), as summarized by the following sentence; ?H2 can be a zero-CO2-emission fuel after combining with O2 from air.? To reduce the greenhouse effect and thus planet?s global warming, one has to reduce CO2 emission from power plants and tail pipes. H2 can be an efficient fuel for consumer vehicles replacing non-sustainable gasoline, but the lightest, inert gas needs to be stored on board and burned (or oxidized with O2) efficiently in a fuel cell. In general, however, those gas molecules are not well controlled for efficient renewable energy applications because of the intrinsic fugacity of gas. To control the fugacity, one has to design a material with enhanced binding sites for gaseous molecules [1-2]. Modern quantum-mechanics-based computations can produce reliable microscopic information about interaction between gas molecules and real materials. Based on such information or lessons from quantum mechanics, we can be able to design a better material with better performance in renewable energy applications. Utilizing this strategy, we have been proposing better hydrogen storage materials such as defect-engineered graphene [3] and metal-organic frameworks [4], a better fuel-cell catalyst [4], and a better carbon dioxide capture material [5]. In this talk, I will discuss details of how we used quantum mechanics information of enhanced gas adsorption in nanostructured materials toward efficient renewable energy applications. [1] Y. Zhao et al., Phys. Rev. Lett. 94, 155504 (2005). [2] Y.-H. Kim et al., Phys. Rev. Lett. 96, 016102 (2006). [3] W. I. Choi et al., Phys. Rev. B 81, 085441 (2010). [4] Y.-H. Kim et al., Phys. Rev. Lett. 105, 236105 (2011). [5] D. H. Lee et al., Phys. Rev. Lett. 106, 175502 (2011). [6] H. C. Choi et al., J. Am. Chem. Soc. 133, 2084≠2087 (2011).