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First principles design of electric-field-assisted high capacity hydrogen storage media[1]

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Hydrogen has been viewed as a highly appealing energy carrier for renewable energy. To achieve economic feasibility hydrogen storage materials with high gravimetric and volumetric densities must be developed. However, no materials so far satisfy the essential criteria for economically feasible hydrogen storage. Therefore, there are necessities of breakthrough ideas and methods for developing new materials. In this talk, I will discuss the novel idea of electric-field-assisted hydrogen storage in nanostructures. Its central ingredient is to create high and strongly delocalized electric fields that are strong enough to attract hydrogen through polarization. Using quantum mechanical first-principles calculations, it has been shown that high electric fields can be easily established in a region close to the surface of nanostructures by electronic doping [1] or in charge compensated ways. The charging idea and its underlying physical mechanism can be generalized to many other related nanoscale materials that are of interest for hydrogen storage, as exemplified by alkaline-earth-metal coated carbon nanostructures [2] and charge transferred organic crystals [3].

[1] M. Yoon, S. Yang, E. Wang, and Z. Zhang, Nano Lett. **7**, 2578 (2007).
[2] M. Yoon, S. Yang, C. Hicke, E. Wang, D. Geohegan, and Z. Zhang, Phys. Rev. Lett. **100**, 206806 (2008).
[3] M. Yoon and M. Scheffler (in preparation).

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