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Functionalized Carbon Nanostructures as Potential Hydrogen Storage Media[1] MINA YOON, The University of Tennessee, Oak Ridge National Laboratory, SHENYUAN YANG, The University of Tennessee, Chinese Academy of Sciences, ENGE WANG, Chinese Academy of Sciences, ZHENYU ZHANG, Oak Ridge National Laboratory, The University of Tennessee — Nanoscaled carbon materials have attracted great attention as promising hydrogen storage media due to their light weight and high surface areas. However, a major limitation is the poor hydrogen uptake resulting from the weak interactions of hydrogen molecules with pristine carbon nanostructures. Recent theoretical studies have investigated ways to increase the binding strength of molecular hydrogen by coating and/or substitutional doping of the carbon nanostructures with transition metals, yet experimentalization of these approaches have been difficult because of metal clustering. In this talk, we study hydrogen storage in carbon nanotubes and fullerenes, by functionalizing such structures with tunable charge states. The tunability is achieved via chemical or electron doping. Our study shows that with the proper method of charge doping, the hydrogen binding strength can be substantially increased. In this way, hydrogen uptake of > 6.0 wt % at ambient conditions can be realized.

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