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Fundamental design of hydrogen storage structures and systems.

ZHENG XIAO GUO, University College London

Fundamental simulations of hydrogen interactions with host structures offer indispensable insights to the understanding and design of hydrogen storage materials for practical applications. First-principles approaches were applied to selected materials of high promise, e.g., doped/defective carbon, doped hydrides and metal/amine complexes. Several candidates show large capacities for hydrogen – over the 6-9 mass-percentage threshold considered for applications. Recent progress on carbon nanostructures show the importance of defects and doping on extra hydrogen uptake, and a small change of C-C interspacing on the mode-switching of hydrogen sorption. Work on the molecular analogues of the basic structural unit of boron-nitride indicates that transition metal (TM) atom doping can boost both the gravimetric and thermodynamic capacities of hydrogen in these materials. The H2 binding to the TM dopants is Kubas-like in nature, though the maximum binding capacity at the TM doped sites does not follow the 18-electron rule. Progress in the Li-N-H system shows that the N-Li bond is weaker than one of the N-H bonds in LiNH2, and consequently LiNH2 can dissociate into: Li+ and (NH2)-, or (LiNH)- and H+. Hence, NH3 may evolve as a transient gas, if it is not sufficiently captured by a reactive component, e.g. LiH. Molecular dynamics calculations indicate that hydrogen deliveries are possible close to fuel-cell operation conditions. Comparison is also made with experiment where possible.