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Design of tailored carbon nanostructures for hydrogen storage[1]
PHILIPPE F. WECK, Chemistry Dept., UNLV, EUNJA KIM, Physics Dept., UNLV, NADUVALATH BALAKRISHNAN, Chemistry Dept., UNLV, HANSONG CHENG, Air Products & Chemicals, Inc. — In a time of increasing scarcity of fossil fuel resources worldwide, hydrogen is widely regarded as a potential cost-effective, renewable and clean energy alternative to petroleum, especially in the transportation sector. However, storage of hydrogen has revealed to be particularly challenging so far. In the present work, we report our progress on the computational study of functionalized carbon nanostructures for hydrogen storage. Structures and properties of these nanostructures consisting of single-walled carbon nanotubes constrained by spacers were calculated using the density functional theory (GGA, PW91). Particular emphasis was given to understanding the role of the chirality and diameter of small single-walled carbon nanotubes on the overall thermal stability and storage capacity of such nano-frameworks.

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