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A theoretical study of the hydrogen-storage potential of $(H_2)_4CH_4$ in nanotubes and MOFs TIMO THONHAUSER, QI LI, Wake Forest University — The material $(H_2)_4CH_4$, also called H4M, has exceptional hydrogen-storage potential of up to 33.3 mass%, not including the hydrogen in CH_4.[1] But, unfortunately, H4M is not stable under ambient conditions. For hydrogen storage near ambient pressure, it needs to be cooled to 65 K, and ambient temperature requires a pressure of 5–6 GPa.[2] In this study we use *ab initio* methods based on van der Waals DFT[3,4] to investigate the possibility of creating such pressures through external agents such as metal organic framework (MOF) materials and carbon nanotubes. We find that MOFs can create considerable pressure for H4M in their cavities, but not the required 5–6 GPa, and therefore moderate cooling is still necessary. On the other hand, carbon nanotubes can create these high pressures for H4M, but the fact that this pressure exists only inside the nanotubes—and not in-between tubes in e.g. a bundle—lowers the volumetric storage density and makes this option less favorable for practical applications.

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[2]W.L. Mao et al., Chem. Phys. Lett. **402**, 66 (2005).
[3]M. Dion et al., Phys. Rev. Lett. **92**, 246401 (2004).
[4]T. Thonhauser et al., Phys. Rev. B **76**, 125112 (2007).

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