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Theoretical study of hydrogen bonding to metal-coated carbon nanotubes[1] JEONGNIM KIM, University of Illinois, Urbana-Champaign, QMCPACK DEVELOPERS TEAM — Dihydrogen transition metal complexes and carbon nanostructures are promising hydrogen storage materials [1]. While the practical storage capacity of pure carbon nanostructures is low, calculations predict a possible hydrogen capacity of above 6 wt.% for Ti coated nanotubes [2]. A unique hybridization of Ti-d, H-H σ^* and carbon π-orbitals was attributed for the bonding; light alkali and alkaline metals were excluded as alternatives to Ti [2]. This is at odd with earlier predictions of non-transition-metal complexes and synthesis of alkali-doped carbon nanotubes (CNT) [1]. Quantum Monte Carlo (QMC) methods are well suited to describe the strong correlation effects tha to the weak hydrogen binding and metal-hydrogen interactions. We present QMC study of hydrogen bonding to metal-coated CNT using correlated umbrella samplings. Specifically, we study hydrogen bonding to Ti and Mg at various doping levels on CNT.

[1] R. C. Lochan and M. Head-Gordon, Phys. Chem. Chem. Phys. **8**, 1357 (2006).
[2] T. Yildirim and S. Ciraci, Phys. Rev. Lett. **94**, 175501 (2005).

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