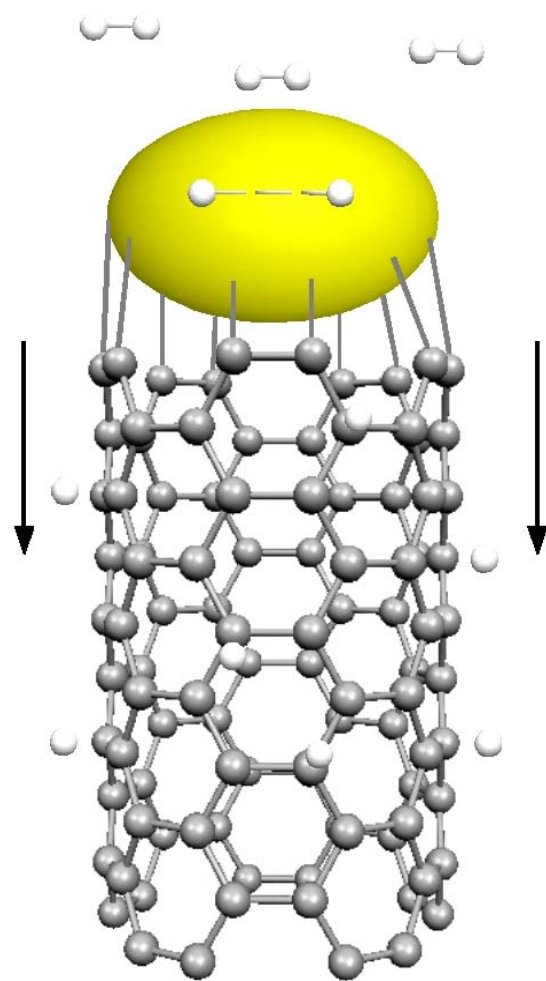


Bill Poirier
Texas Tech University
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PI Professor Bill Poirier and coworkers at Texas Tech University, are the first to elucidate a fundamental mechanistic understanding of the spillover process for hydrogen storage via (single-walled) carbon nanotubes (SWNTs), using a comprehensive first principles treatment incorporating curvature, corrugation effects, accurate electronic structure, and quantum dynamics. All are found to play an important role.

Hydrogen storage via “spillover.” The catalyst (yellow oval) binds to the top of the (5,5) SWNT substrate. Five unit cells are indicated. Molecular hydrogen enters from the top, and is dissociated by the catalyst. The resultant H atoms “spill over” on to the SWNT substrate, and migrate downwards. The entire process is experimentally found to be reversible.