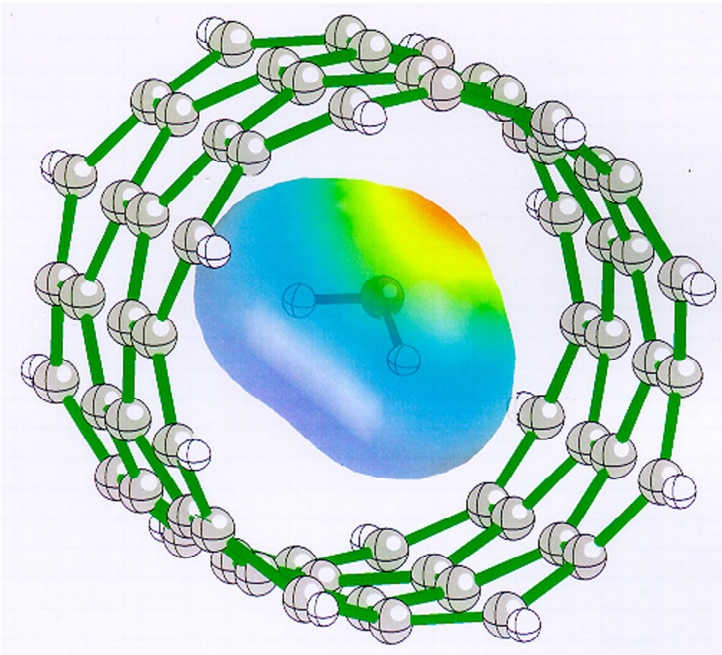
GC-2 Highlight

U. Pittsburgh, EMSL

Computational Thermochemistry and Benchmarking of Reliable Methods



Due to the lack of experimental information, the development of a reliable empirical force field for molecular dynamics simulations capable of describing water inside of a carbon nanotube requires input from theory. To this end, we have carried out large basis set, perturbation theory calculations on a single water molecule bound to fused benzene ring systems up to $C_{96}H_{24}$ (representing planar graphite). The water/graphite electronic binding energy was estimated to be -5.8 ± 0.4 kcal/mol. This is very similar to the value of 5.0 ± 0.1 kcal/mol found for the water dimer.

Similar calculations on water within a short segment of a nanotube are currently underway.

"Estimating the Strength of the Water/Single-Layer Graphite Interaction", D. Feller and K. D. Jordan, J. Phys. Chem. A **104**, 9971(2000).

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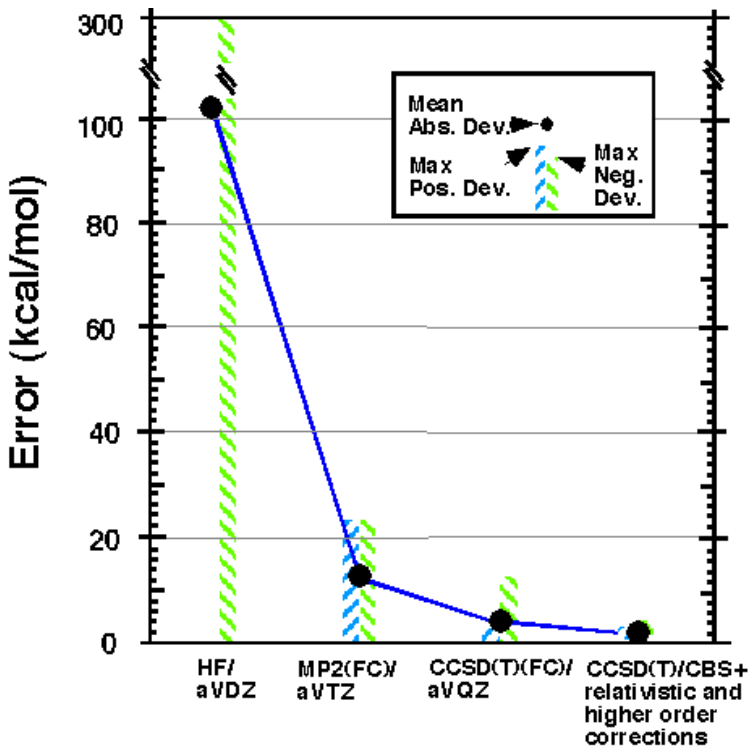

The ability to accurately predict a variety of thermochemical data is critical to a wide range of technological problems, including the development of environmentally benign materials and chemical processes. Experimental techniques for measuring these quantities are frequently prohibitively expensive compared to computer models. Although the area of computational thermochemistry is an extremely active one, most researchers have elected to incorporate one or more empirical parameters into their models, which can potentially limit their accuracy and scope. We are developing a high-level ab initio approach designed to incorporate all effects in order to obtain ~1 kcal/mol accuracy without the use of empirical parameters.

"Predicting the Heats of Formation of Model Hydrocarbons up to Benzene", D. Feller and D.A. Dixon, *J. Phys. Chem. A* **104**, 3048 (2000).

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