Accurate *ab initio* studies of hydrocarbon physisorption on carbon nanotubes

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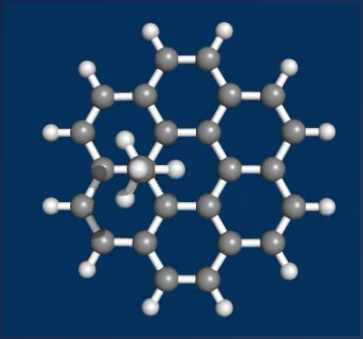
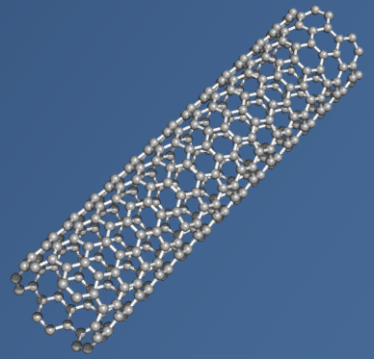
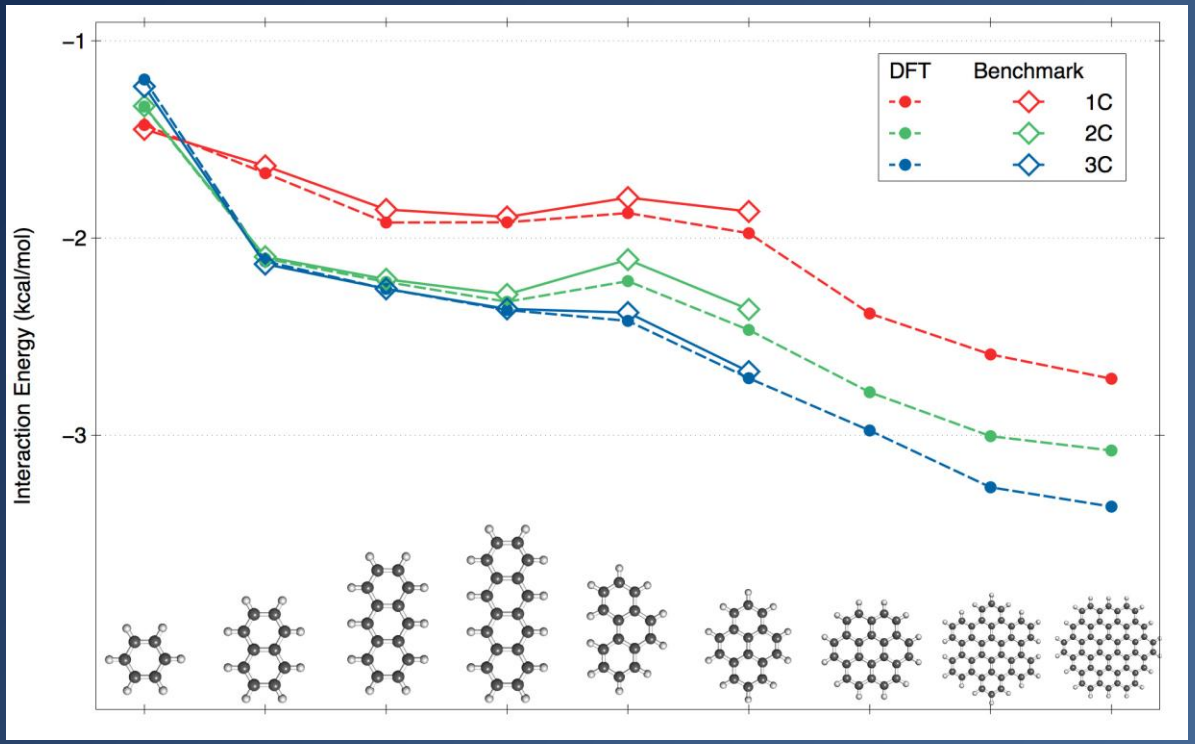


Carbon nanotubes – "materials of the 21st century"

- strong and durable scaffolding
- tunable electrical and optical properties
- can adsorb molecules (hydrogen, carbon dioxide, methane)

natural gas storage, transport, sensing, and catalytic combustion





Goal: to develop improved adsorption potentials for methane on graphene and carbon nanotubes

Stage 1: we obtained highly accurate benchmark energies for model dimers of methane with polycyclic aromatic hydrocarbons

Stage 2: we identified an accurate and efficient DFT algorithm to calculate interaction energies for larger dimers

Ongoing work

- even larger model dimers
- infinite systems
- curvature effects