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