Session #1: Cutting Edge Methodologies (beyond Current DFT)

Moderator: *Shengbai Zhang (RPI/NREL)*

Topics to be addressed: Benchmarking state-of-the-art approaches, accurate energy landscape. Identify problems with the current DFT-LDA and GGA approaches and possible pathways to overcome these problems.

How Bad is DFT for vdW Interactions?

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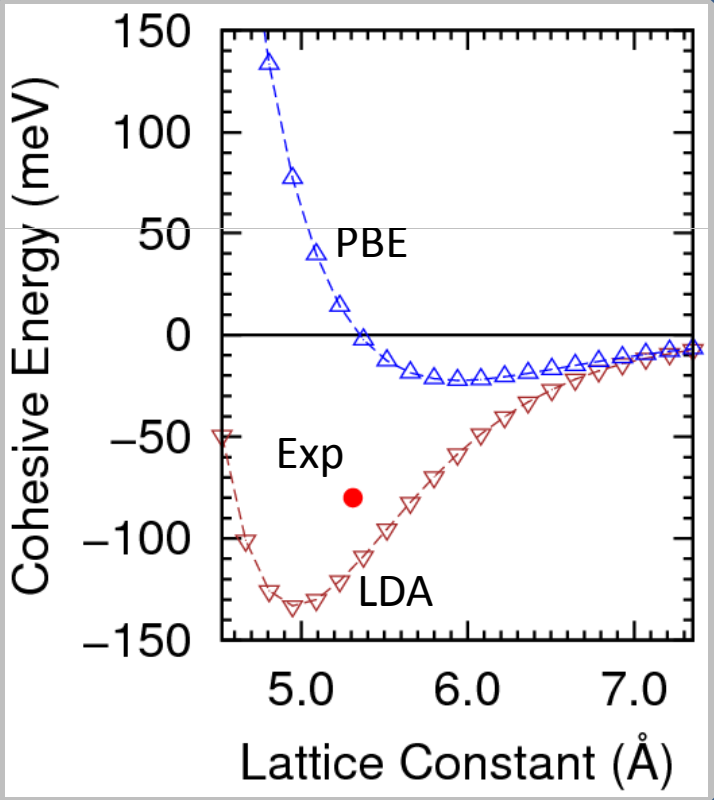
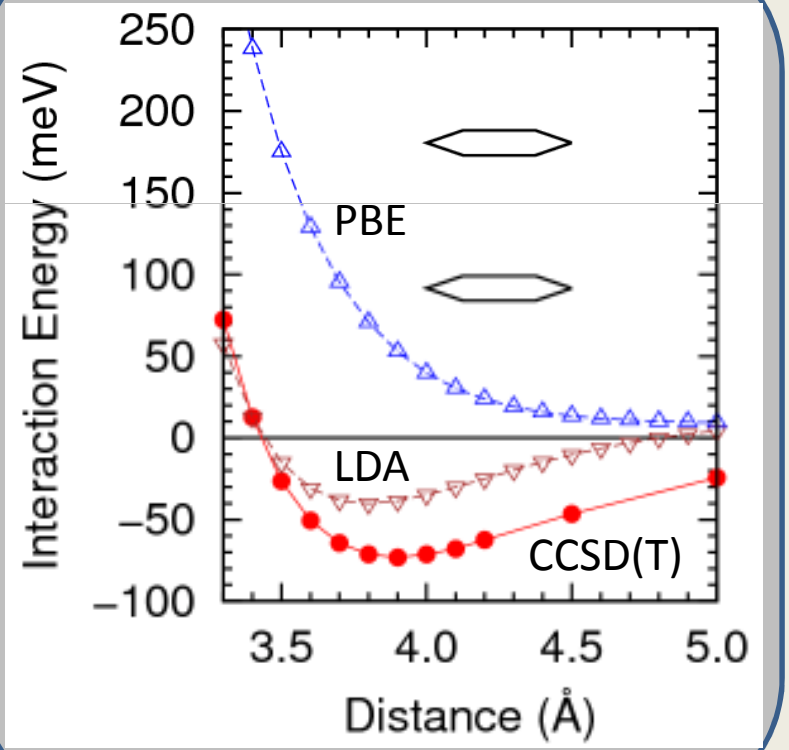
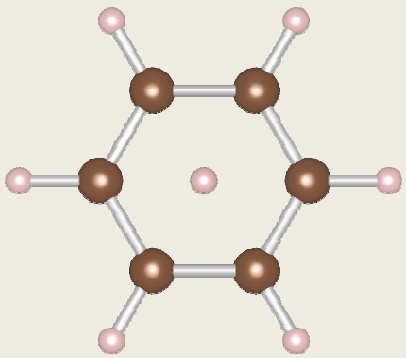
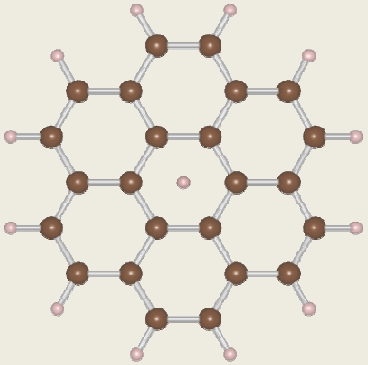


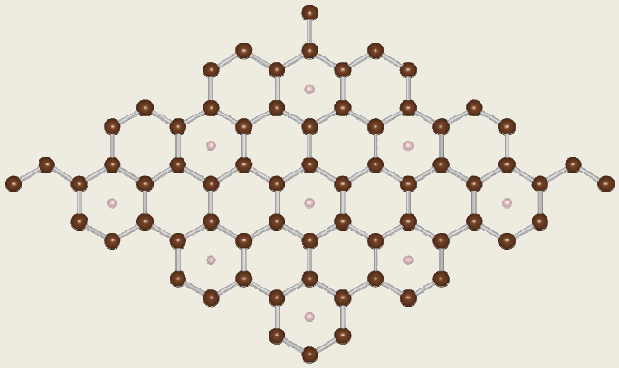
Benzene dimer

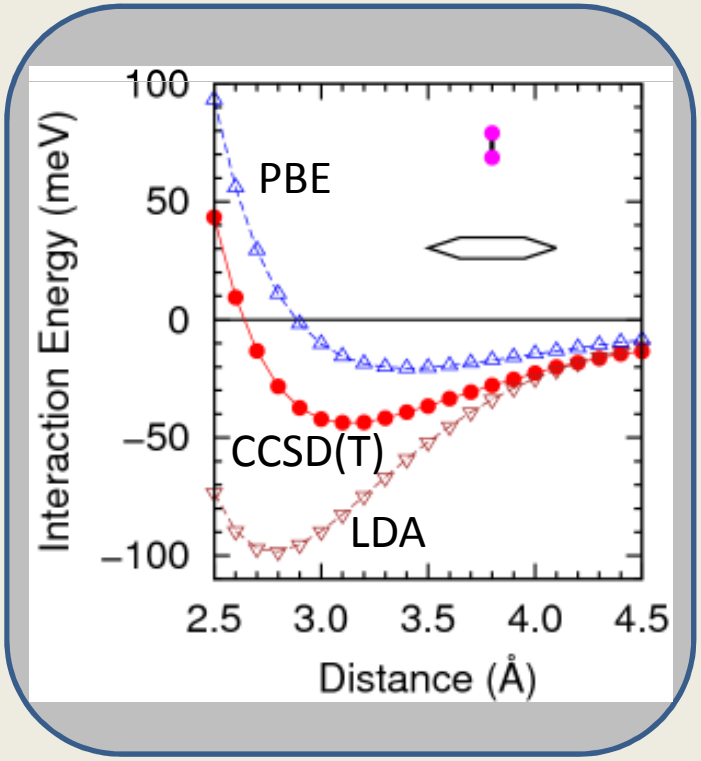


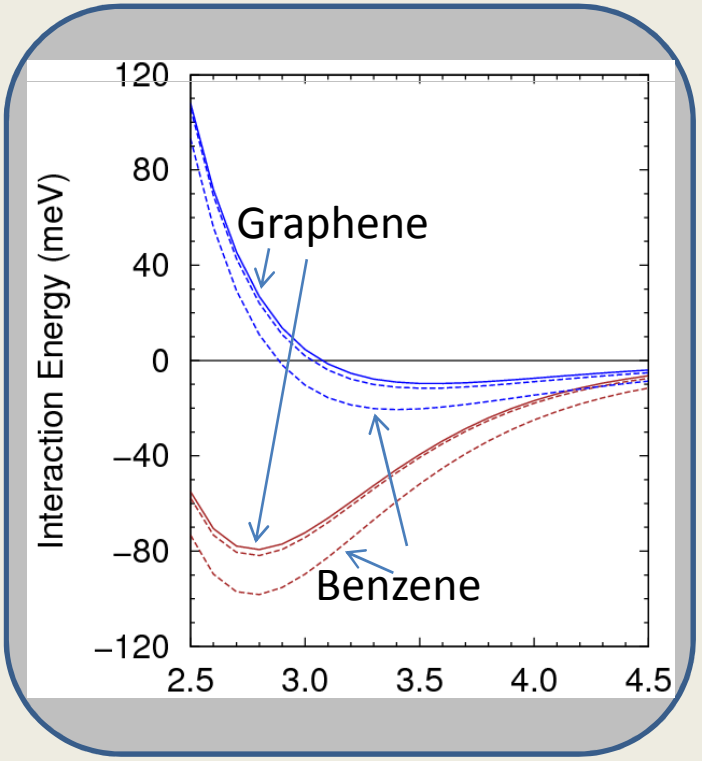
vdW Interaction between H_2 and Carbon











van der Walls (vdW)-DFT: *Langreth, Kohn*

Fully nonlocal functional:

$$E_c^{nl} = \frac{1}{2}\int d^3r\, d^3r'\, n(\vec{r})\phi(\vec{r},\vec{r}\,')n(\vec{r}\,')$$

- Long-range nonlocal correlation energy functional (omitted in the LDA and GGA)
- Computational cost considerably more than GGA
- Added as post-GGA energy correction but force calculation is still expensive.

*S1.3 Langreth, Tuesday, 9:00 AM (Rm 3008, Moscone West)
*S5.5 Morikawa, Thursday, 10:15 AM

A Local Potential Approximation to vdW-DFT

S1.8 Sun, Tuesday, 11:30 AM

*S4.4 Kim, Wednesday, 2:45 PM

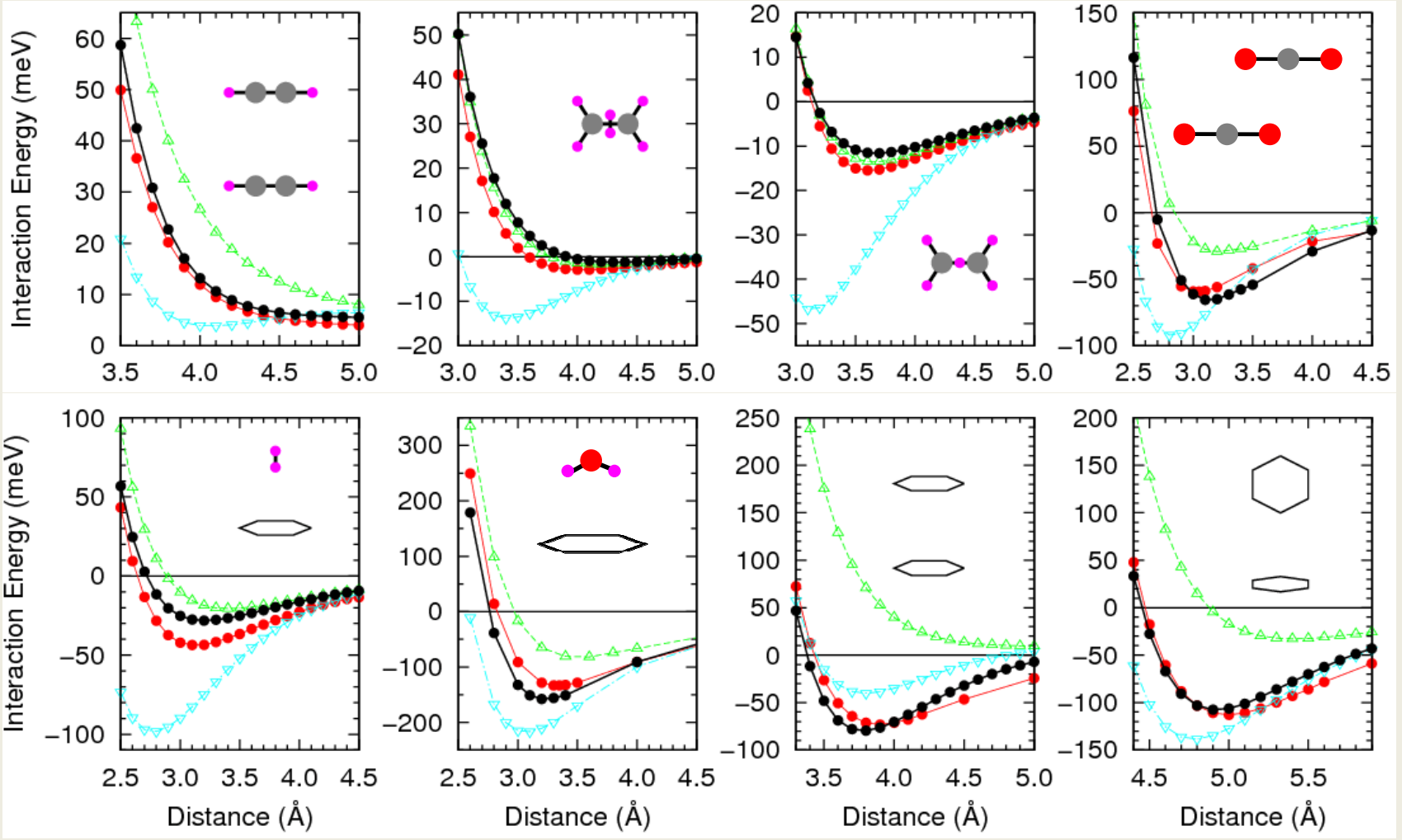
$$V^{\mathrm{vdW}}(\mathbf{r}) = \frac{\delta E^{\mathrm{vdW}}[n]}{\delta n}$$

$$\{T + V^{\mathrm{H}} + V^{\mathrm{ext}} + V^{\mathrm{xc}} + V^{\mathrm{vdW}}\}\psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r})$$

$$\approx \sum_i v(|\mathbf{r} - \mathbf{R}_i|)$$

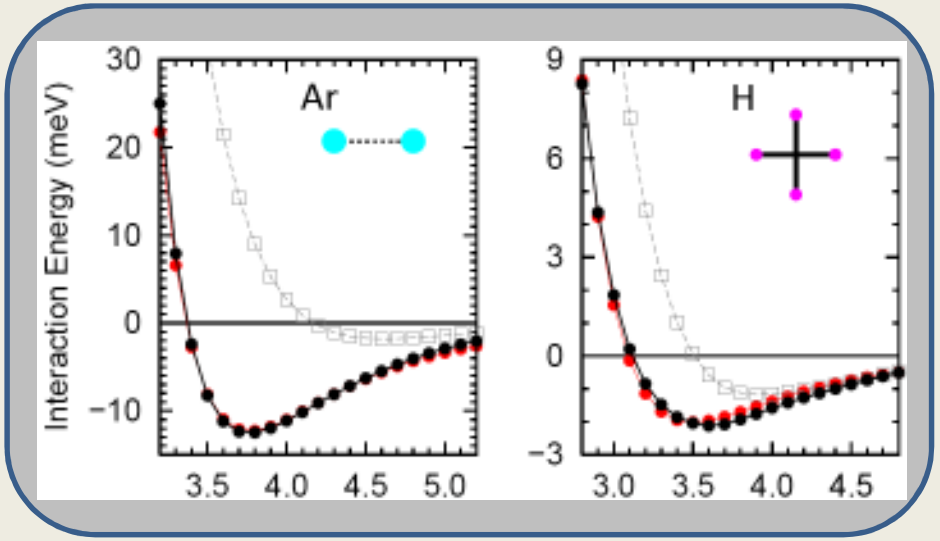
- Deriving local potentials by fitting to CCSD(T) energy curves: *simple, straightforward, and once for all.*

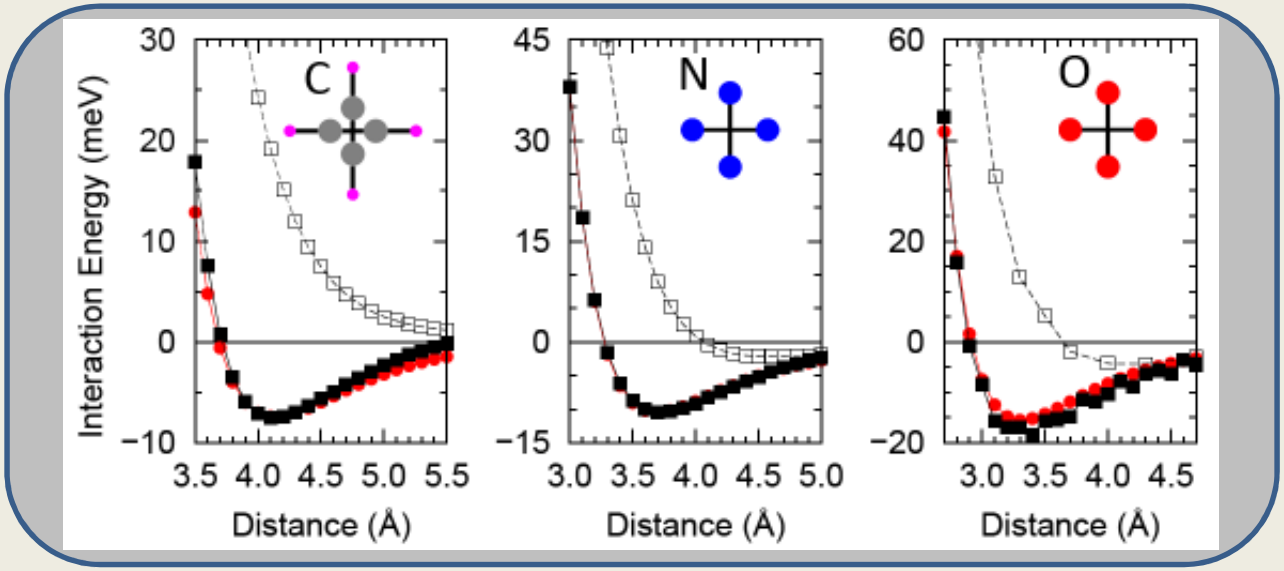
Testing Local Atomic Potential Approach



Generating Local Atomic Potentials (LAPs)

$$v(r) = \begin{cases} -\frac{c_0}{r^n} & \text{if } r > r_{\text{cut}} \\ v_{\text{const}} & \text{if } r \leq r_{\text{cut}} \end{cases}$$





revPBE

LAPs

CCSD(T)

Testing LAPs on Periodic Systems

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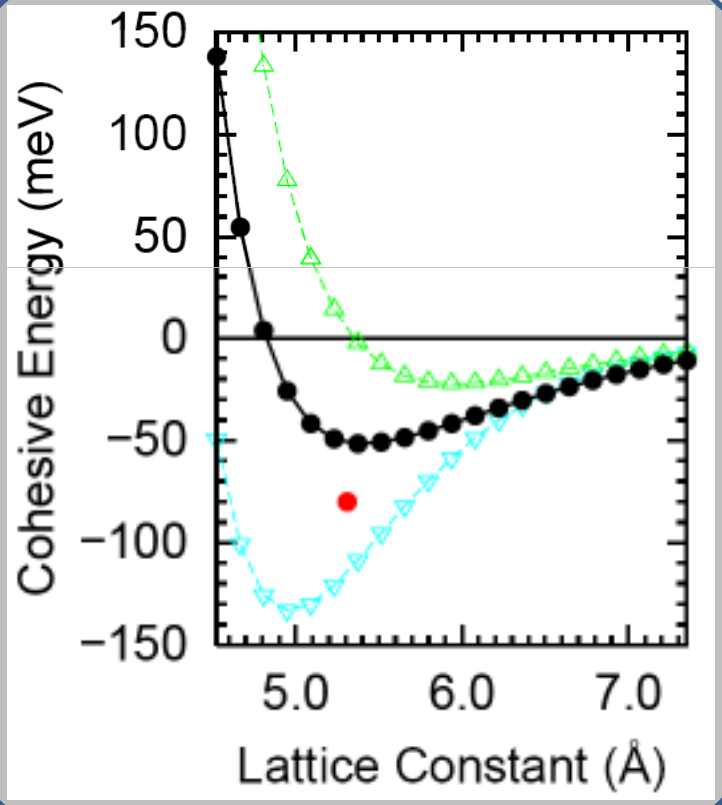

Adenine on graphene