Data Review

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Intermolecular Energies

- Supermolecular approach

$$E_{int} = E_{AB} - E_A - E_B$$

  - Straightforward, but cannot separate different types of interactions
  - Can adopt to different electronic structure methods
  - DFT-D3 with proper functional can be both cheap and accurate
- Symmetry-Adapted Perturbation Theory
  - Can give details about different types of interactions; important in understanding their nature
  - Not as cheap as DFT-D3
  - SAPT0 is somewhat cheap, but does not include intramonomer correlation

SAPT(DFT)

- Attempt to inlude intramonomer correlation in a cheap way
- Replaces HF orbitals with KS orbitals
- Needs to consider orbital response for dispersion terms
- Exchange-dispersion term needs to be estimated from scaling
- Investigate the accuracy and efficiency of SAPT(DFT)

Three-Body Interaction

- Crucial in computing lattice energies
- DFT-D3 does not perform well for three-body interaction
- MP2.5 scales as $O(N^6)$, MP2 $O(N^5)$ but lacks three-body dispersion
- Three-body dispersion can be implemented with SAPT(DFT) in $O(N^5)$

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Idea of SAPT(DFT)

- SAPT energy in orders of interaction and fluctuation potentials; n denotes order in V and k, l for W_A, W_B

$$H = F_A + F_B + V + W_A + W_B$$

$$E_{int} = \sum_{n=1}^{\infty} \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \left(E_{pol}^{(nkl)} + E_{exch}^{(nkl)} \right)$$

- SAPT0: $n = 2, k = l = 0$, no intramonomer correlation, $O(N^5)$ cost
- Many-body SAPT: $k, l \geq 2$, $O(N^7)$ or higher cost
- SAPT(DFT): Use Kohn-Sham operator $K_{A,B}$ instead of Fock operator $F_{A,B}$, $O(N^5)$ cost
- Primitive SAPT(DFT) works well on 1st-order terms but not 2nd-order terms (especially dispersion terms), needs orbital response for them

Dispersion Term

$$E_{disp}^{(2)} = -\sum_{m\neq 0, n\neq 0} \frac{\left|\langle \Psi_0^A \Psi_0^B | V_{AB} | \Psi_m^A \Psi_n^B \rangle\right|^2}{E_m^A - E_0^A + E_n^B - E_0^B} \quad (1)$$

$$= -4 \sum_{ia\in A, jb\in B} \frac{\left|\left(i^A a^A | j^B b^B\right)\right|^2}{\epsilon_a^A - \epsilon_i^A + \epsilon_b^B - \epsilon_j^B} \quad (2)$$

- ALDA kernel good for pure GGA functional but not for hybrid functional
- Exact exchange in $v_{xc} \rightarrow$ increased $\epsilon_{ij}^{ab} \rightarrow$ decreased $E_{disp}^{(2)}$
- Either hybrid ALDA kernel or localized HF (LHF) exchange to compensate

$$f_{xc} = \alpha f_{xc}^{HF} + (1-\alpha) f_{xc}^{ALDA}$$

Test 5

Test0	Test1	Test2
Test1	Test2	Test3 LaTeX
Test4	Test5	Test6

Test 6

Example block

Test0	Test1	Test2
Test1	Test2	Test3 LaTeX
Test4	Test5	Test6

Block

Test0	Test1	Test2
Test1	Test2	Test3 LaTeX
Test4	Test5	Test6

Test 7

Block A

short	Short stuff
long	Longer stuff
longest label	Longest stuff (insert cat)

- item1
- item2
- item3

Frame with Columns

Block 1

Text here

Block 2

More text here

Frame without Columns

Block

Even more text here