Data Review

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Table of contents

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 $O(N^5)$

Table of contents

Table of contents

Introduction

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

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

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

- Different truncation for various SAPT levels, $k, l \geq 2$ for intramolecular correlation, introduces expensive cross-term with order $(n + k + l)$
- Cheap intramolecular correlation with SAPT(DFT), use Kohn-Sham operator $K_{A,B}$ instead of Fock operator $F_{A,B}$ and $k, l = 0$
- Primitive SAPT(DFT) or SAPT(KS) works well on 1st-order terms but not 2nd-order terms (induction, dispersion), needs orbital response for them

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