pyfragment Documentation

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BACKGROUND

PyFragment is a collection of Python modules that facilitate the setup and parallel execution of *embedded-fragment* calculations on molecular clusters, liquids, and solids.

1.1 Theory

The *embedded-fragment* methods are rooted in the many body expansion (MBE), which expresses the total energy of a molecular system as

$$E = \sum_i E_i$$

drivers.**energy_driver**()
SP energy

1.2 Implementation

A series of modules are available. Please check:

1.2.1 Codes

class ChargeState.**ChargeState**(*fragments*, *fragment_charges*)
Base class for VB CT state

coupling_dimer_gs(*state2*, *embed_flag=None*)
-sqrt([E_(AB)+ - E_(A+B)]*[E_(AB)+ - E_(AB+)]) E_(AB)+ == the relaxed, correlated charged dimer E_(A+B) == non-stationary HF energy of the charge-local dimer

plus monomer correlation energies of E_A+ and E_B

For a dimer system, this method reproduces the exact E by construction

coupling_dimer_gs_no_embed(*state2*)
Wraps the above dimer_gs coupling, but the two monomers do not polarize each other in monomerSCF. Hence, it does not exactly reproduce the dimer GS energy by construction

coupling_dimer_gs_overlapHOMO(*state2*)
S*E_(AB)+ - sqrt([E_(AB)+ - E_(A+B)]*[E_(AB)+ - E_(AB+)]) Second term is same as coupling_dimer_gs First term is overlap of monomer HOMO's times relaxed dimer energy This method also reproduces energy of a dimer by construction; it just makes the overlap matrix non-identity

diag_chargelocal_dimers(*subcomm=None*)

return E1 + E2, the BIM energy of this charge-transfer configuration E1: sum of monomer correlated energies E2: sum of dimer interaction energies (E_AB - E_A - E_B)

interaction INCLUDES correlation for relaxed dimers (when A&B have same charge) but it's just the non-stationary HF energy for charge-local dimers

CHAPTER

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