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 (under construction...)

$$E = \sum_i E_i$$

1.2 Implementation

Under construction...

1.2.1 Codes

Under construction

CHAPTER

TWO

THE GLOBALS MODULE

globals contains essential shared data and functionality for *all* types of fragment calculations.

2.1 globals.geom

Defines the fundamental Atom class to conveniently load and print geometry information. Contains functions for loading geometry and performing *fragmentation*, that is, assigning which atoms belong to which fragments.

class globals.geom.**Atom**(*atomstr*, *units='angstrom'*)
Convenience class for loading and storing geometry data

globals.geom.**load_geometry**(*data*, *units='angstrom'*)
Builds geometry from input text, lists, or filename.

Tries to be flexible with the form of input 'data' argument. Uses regex to extract atomic coordinates from text.

Args:

data: string, list of strings, list of lists, or filename containing the xyz coordinate data

units (default Angstrom): "bohr" or "angstrom"

Returns: geometry: a list of Atom objects

globals.geom.**makefrag_auto**(*geometry*)
Auto-generate list of fragments based on bond-length frag_cutoffs.

Use this if you don't wish to manually assign atoms to fragments.

Args: geometry: list of Atom objects

Returns: fragments: a list of fragment atomic indices

globals.geom.**makefrag_full_system**(*geometry*)
No fragmentation: all atoms in system belong to one fragment.

Use this to perform one big reference QM calculation

Args: geometry: list of Atom objects

Returns: fragments: a list of fragment atomic indices

globals.geom.**nuclear_repulsion_energy**(*geometry*)
Nuclear repulsion energy, hartrees

CHAPTER

THREE

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