Version 1.1.0

Written by Nathan Bamberger

List of Main Analysis Functions

Functions which are not intended to be directly called by the user are not included in this list. For a detailed description of every input and output of a function, see the header at the top of its .m file.

- rotate_mol_to_align_axis
  - Rotates a set of atomic coordinates in space so that the line between two specified atoms lies along the x-axis, centered at zero.
- PlotAtomCoords
  - Creates a plot showing the atomic symbol for each atom at its specified coordinates.
- Display_ChargeElectrode_System
  - Creates a plot representing the sign and relative magnitude of all partial charges on the molecule, along with the specified number of sets of charge images inside the two electrodes.
- SingleGapSize_ImageChargeCalculation
  - Calculates the total image charge renormalization energy for a given partial charge distribution at a single specified gap size (and also shows the convergence of that energy as more and more image charge iterations are added).
- ImageChargeCalculation_GapSizeSweep
  - Calculates how the total image charge renormalization energy for a given partial charge distribution varies as the gap size changes.
- Detailed_TwoElectrode_Renormalization
  - At a single gap size, calculates how much different specific pair-wise interactions contribute to the total image charge renormalization energy for a given partial charge distribution.
- DifferenceInPartialCharge_PerAtom
  - Given two similar molecules, qualitatively displays the difference in partial charge on each conserved atom.
- match_up_atoms
  - Given two similar molecules, finds the rotation in which they best align with each other and uses that overlap to determine which atoms are “conserved” between the two and which atoms are specific to one molecule or the other.
- DifferenceInRenormEnergy_PerAtom
  - Given two similar molecules, qualitatively displays the difference in the contribution of each conserved atom to the total image charge renormalization energy.
- CompareDetailed_TwoElectrode_Renormalization
  - Given two similar molecules, quantitatively shows the difference in the contribution of each conserved atom to the total image charge renormalization energy.

- CompareDetailed_TwoElectrode_Renormalization_2D
    - Given two similar molecules, quantitatively shows the difference in the contribution of different pair-wise interactions to the total image charge renormalization energy.
- ImageRenorm_DuringRotation
    - Calculates how the total image charge renormalization energy for a given partial charge distribution varies as the molecule is rotated inside the electrode gap.
- DisplaySystem_SphericalElectrodes
    - Displays the electrode-charge system in the case of spherical electrodes
- SingleGapSize_RenormEnergy_SphericalElectrodes
    - Calculates the total image charge renormalization energy at a single gap size, in the case of spherical electrodes (and also shows the convergence of that energy as more and more image charge iterations are added).
- ImageChargeCalculation_GapSizeSweep_SphericalElectrodes
    - Calculates how the total image charge renormalization energy for a given partial charge distribution varies with the gap size between two spherical electrodes