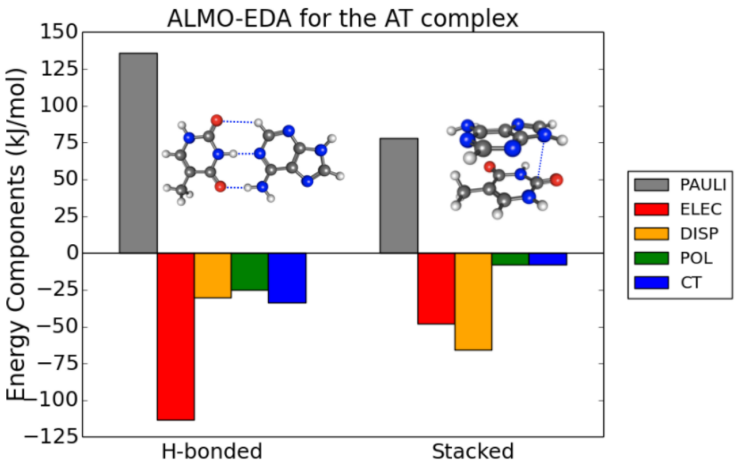
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Absolutely Localized Molecular Orbitals Based Energy Decomposition Analysis (ALMO-EDA) for Intermolecular Binding Interactions



- DFT-based ALMO-EDA allows users to:
  - Quantify the following contributions to intermolecular binding energy:
    - Permanent electrostatics (ELEC);
    - Pauli repulsion (PAULI);
    - Dispersion (DISP);
    - Polarization (POL);
    - Charge-transfer (CT);
    - Solvation energy (when implicit solvent model is used).
  - Analyze shifts in complex's structural and vibrational properties through geometry optimization and harmonic frequency analysis on each intermediate potential energy surface.
- Useful ALMO-EDA extensions:
  - DFT-based ALMO-EDA for bonded interactions;
  - ALMO-EDA for second-order Møller-Plesset perturbation theory;
  - ALMO-EDA for interactions involving excited state molecules described by TDDFT/TDA.

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