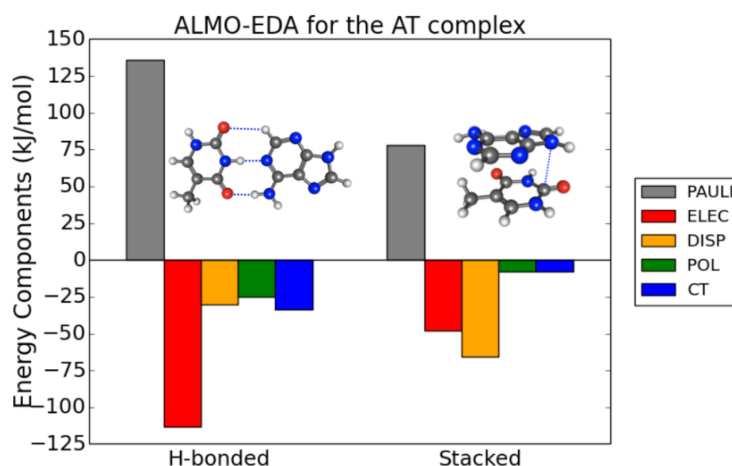


Absolutely Localized Molecular Orbitals Based Energy Decomposition Analysis (ALMO-EDA) for Intermolecular Binding Interactions



- 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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