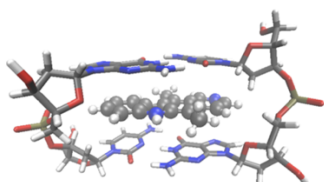
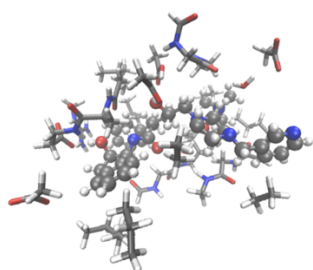


Extended Symmetry-Adapted Perturbation Theory (XSAPT)



DNA / ellipticine



HIV / indinavir

Method	E_{int} (kcal/mol)	
	DNA/ellipticine	HIV/indinavir
B97M-V (+counterpoise) ^a	-41.3	—
ω B97M-V (+counterpoise) ^a	-43.7	—
HF-3c	-41.7	-132.8
PBEh-3c	-37.3	-119.1
XSAPT+ <i>ai</i> D3 (CM5) ^b	-36.7	-106.2
XSAPT+MBD (CM5) ^b	-41.7	-125.4
XSAPT Energy Decomposition		
E_{elst}	-22.2	-114.9
E_{exch}	59.2	190.0
E_{ind}	-8.0	-65.9
E_{disp}	<i>ai</i> D3+ATM	-65.7
	MBD+esDQ	-70.7

^adef2-TZVPPD basis set. ^bdef2-hpTZVPP basis set

XSAPT+*ai*D Interaction Energies and Energy Decomposition Analysis

- Benchmark-quality intermolecular interaction energies;
- Energy decomposition analysis provides a powerful interpretive utility;
- Unfolds interaction energies into contributions from electrostatics, Pauli repulsion, polarization, and London dispersion;
- A fully many-body interaction energy protocol:
 - Accounts for many-body polarization effects via charge embedding;
 - Includes many-body dispersion interactions (MBD+esDQ potential).
- Cost scales with monomer size; no need for supersystem calculations;
- Faster than supersystem DFT for the DNA complex shown above (4,651 basis functions);
- Trivially parallelizable across fragments;
- Capable of high-accuracy interaction energies in systems larger than 10,000 basis functions.

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