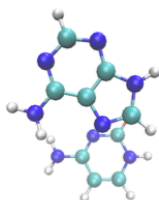


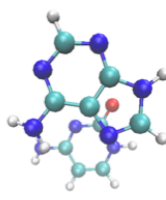
# Impact of geometry optimization on base-base stacking interactions: An energy decomposition analysis

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## Top view of CA stacked dimer

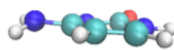
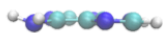


A-form

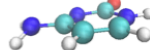
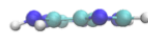


B-form

## Side view of CA stacked dimer



A-form



B-form

Deoxyribonucleic acid (DNA) exists in multiple right-handed double helix conformations, including A- and B- forms; B-form typically exists in aqueous solution, while A-form exists in low water activity solutions, such as solutions with high salt or ethanol concentrations. The differences in the conformations of both A- and B- form DNA affects the energetics of the helix, including base stacking. Previous work has demonstrated the importance of geometry optimization in determining base stacking energies in A-form and B-form DNA. In this work, we use symmetry-adapted perturbation theory (SAPT) to analyze the energy contributions to the overall stacking energies for all possible DNA base stack sequences. The sequence dependence of changes in the energy contributions is analyzed. Further, analysis of the components of the interaction energy provides insight into the physics of base stacking interactions in both A- and B- form DNA. Finally, possible correlations between the components of the interaction energy and the total interaction energy, and correlations between the geometry of the base stacks and the components of the interaction energy are considered.