Intermolecular Non-Covalent Interactions in π-Conjugated Heterocyclic Oligomers

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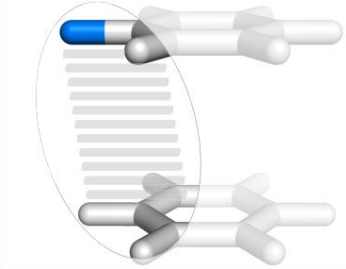
Local, Direct Interaction Model



Substituent effects in π-stacking interactions arise from direct interactions between the substituents and the other ring, not any effects involving the aryl π-system

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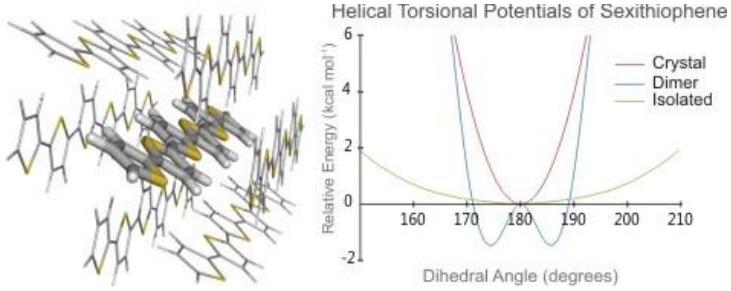
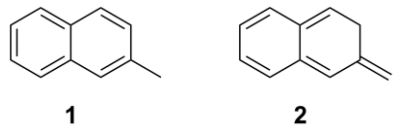
Impact of Neighboring Chains on Torsional Potentials of Oligothiophenes

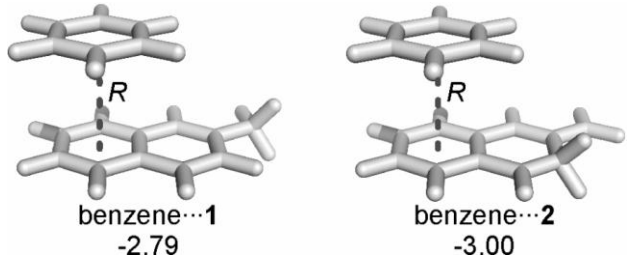


Interactions with neighboring have a dramatic impact on computed torsional potentials of sexithiophene, and must be accounted for to accurately predict the physical properties of these common components of organic electronic materials.

Role of Aromaticity in π-Stacking Interactions



1 aromatic **2** non-aromatic



In contrast to prevailing assumptions, romaticity is not only unnecessary for π-stacking interactions, but actually hinders many of these non-covalent interactions.

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