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Controlling Conformations of Conjugated Polymers and Small Molecules: The Role of Nonbonded Interactions KEVIN KOHLSTEDT, NICHOLAS JACKSON, BRETT SAVOIE, LIN CHEN, MONICA OLVERA DE LA CRUZ, GEORGE SCHATZ, MARK RATNER, Northwestern University — The chemical variety present in the organic electronics literature has motivated us to investigate potential nonbonding interactions often incorporated into conformational "locking" schemes. We have examined a variety of potential interactions, including oxygen-sulfur and nitrogen-sulfur, using accurate quantum-chemical wave function methods on a selection of high-performing conjugated polymers and small molecules. In addition, we evaluate a set of nonbonding interactions occurring between various heterocyclic and pendant atoms taken from a group of representative pi-conjugated molecules. From our survey, it is determined that while many nonbonding interactions possess weak binding capabilities, hydrogen bonding interactions, namely oxygen-hydrogen and nitrogen-hydrogen, are alone in inducing conformational control and enhanced planarity along a polymer or small molecule backbone at room temperature.

Kevin Kohlstedt
Northwestern University

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