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Intermolecular bonding in conjugated polymers JEREMY D. SCHMIT, University of California, Santa Barbara, ALEX J. LEVINE, University of Massachusetts, Amherst — Soluble conjugated polymers may enable the development of fast sensitive biosensors. However, the tendency of these molecules to aggregate even at low concentrations has a profound effect on the fluorescence signal that these sensors rely on. We propose that the aggregation of doped conjugated polymers occurs due to the formation of weak interpolymeric bonds resulting from intermolecular electron tunneling at crossing points of the chains. Although these bonds are essentially covalent in character, they are significantly weaker ($\sim 2k_BT$) due to poor the intermolecular overlap of the electron wavefunctions as well as the delocalization of the pi-electrons along the polymer backbone. We show that the aggregates resulting from these bonds form either loosely bound braids or tight bundles of parallel chains depending on the strength of the electrostatic repulsion between the polymers. Surprisingly, we find that undoped polymers are unable to form parallel bundles. We also explore the interaction of SSH solitons on the chains with these intermolecular binding sites and demonstrate a roughly a four-fold enhancement of the binding strength when each chain has a soliton at the binding site.

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