**Towards Molecular Simulation of Polythiophene Oligomers**

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Quantum-mechanics calculations and molecular simulations have been conducted for a series of thiophene and alkyl-substituted thiophene oligomers. The long-term goal of this research is to examine, through molecular modeling, the impact of multiple chain (or "aggregation") effects on thermochromic properties of poly(3-alkylthiophenes). Initial aspects of this research focus on adding an alkyl side chain to the thiophene oligomer and its effects on physical properties and simulation parameters, such as partial charges. For oligomer or chain assemblies, we are examining the effects of side chain spacing and position correlations on the extent of coplanarity among sequential thiophene rings. Compared to previous studies, this work includes temperature-dependent effects of amorphous regions on property predictions.