An active space electronic structure study of isoquinoline and thiophene

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Isoquinoline and thiophene are two heterocyclic aromatic molecules with broad applications in efficient energy. Consequently, the electronic structure of these compounds is of significant interest. These systems commonly have low-lying excited states of π-π^*, π-σ^*, and n-π^* character, states which are hard to describe without high-level multi-configurational approaches. Here, I will present our recent Complete-Active-Space Self-Consistent-Field (CASSCF) calculations on isoquinoline and thiophene. An important emphasis will be placed on discussing the excited state ordering in isoquinoline. I will also show how our calculations complement gas-phase spectroscopy experiments that have been conducted on isoquinoline. Additionally, I will discuss several future research directions for these aromatic systems.