A minimal model for antiferromagnetism, charge-disproportionation, valence bond solid formation and superconductivity in the charge-transfer solids \( \kappa-(ET)_2X \) and \( Z-[Pd(dmit)_2]_2 \)

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The minimal model most commonly assumed for \( \kappa-(ET)_2X \) and \( Z-[Pd(dmit)_2]_2 \) is an effectively \( \frac{1}{2} \)-filled band frustrated Hubbard model. In this talk I first review the properties of this model, which has antiferromagnetic (AFM), metallic, and quantum spin liquid phases. Mean-field calculations also find a superconducting (SC) phase. Correlated calculations however do not find long-range SC order or a valence-bond solid phase as occurs as in \( Z=EtMe_3P \).

These failures of the \( \frac{1}{2} \)-filled band effective model as well as recent experimental results which suggest that intra-dimer charge degrees of freedom are significant suggest that the minimal model for these systems must include individual molecules rather than their dimers as “sites” and hence be \( \frac{1}{4} \)-filled. I present computational results for a \( \frac{1}{4} \)-filled band Hubbard model on the full monomer lattice of \( \kappa-(ET)_2X \). For weak frustration our calculations find AFM order in agreement with the \( \frac{1}{2} \)-filled band model. Importantly, no charge disproportionation is required within the \( \frac{1}{4} \)-filled band to realize AFM order. In the strongly frustrated region of the phase diagram singlet excited states occur below the lowest triplet. The presence of low-energy singlet states in this strongly frustrated system is reminiscent of the AFM Heisenberg model on the kagome lattice. I discuss the low temperature properties of \( \kappa-(ET)_2Cu_2(CN)_3 \) in view of the above developments.

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