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The effective half-filled band model is inappropriate for the dimerized 2D organic superconductors[1] NILADRI GOMES, University of Arizona, R. TORSTEN CLAY, Mississippi State University, SUMIT MAZUMDAR, University of Arizona — The antiferromagnetism in κ-$(ET)_2X$ can be understood within the effective $\frac{1}{2}$-filled band anisotropic triangular lattice Hubbard Hamiltonian for strong anisotropy. DMFT theories have claimed antiferromagnetic-to-superconductor transition within the same model, as the anistropy is reduced. In previous work we have shown the absence of superconductivity within the triangular lattice $\frac{1}{2}$-filled band Hubbard model for any Hubbard U and any anisotropy. Other DMFT approaches theories have claimed superconductivity within the so-called Hubbard-Heisenberg model, which incorporates an additional antiferromagnetic spin-exchange over and above that due to the Hubbard U. Very recent work has also claimed a valence-bond solid (VBS) phase within the Hubbard-Heisenberg model, which would seemingly explain the observed VBS phase in $EtMe_3P[Pd(dmit)_2]_2$. We report exact calculations that show that neither the VBS nor the superconducting phase occur within the Hubbard-Heisenberg model, showing clearly that the effective $\frac{1}{2}$-filled band model is unsuitable for describing the complete phase space of the κ-$(ET)_2X$. Our work raises serious doubts about the DMFT theories of superconductivity of metal intercalated C_{60} and picene.

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