

Abstract Submitted
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Correlated model calculations of β phase organic superconductors¹ R. TORSTEN CLAY, Mississippi State Univ, S. MAZUMDAR, University of Arizona — The quasi-two-dimensional organic charge-transfer salts of the β and β' structures display a wide range of electronic behavior including anti-ferromagnetism (AFM), charge ordering (CO), and superconductivity (SC). In the temperature-pressure phase diagram, CO is found adjacent to SC. In the β structure stacks of $\frac{3}{4}$ -filled (one half hole per molecule) organic molecules are strongly dimerized. The presence of CO adjacent to SC is of particular interest as one carrier per dimer gives an effectively half-filled band that should instead favor AFM. We show that the charge ordered state evolving into SC in these materials is a Paired Electron Crystal, with singlet formation between dimers giving a spin gap simultaneous with charge order. We present the results of calculations within a two-dimensional $\frac{3}{4}$ -filled Hubbard model using the Path Integral Renormalization Group (PIRG) and quantum Monte Carlo methods. Our results demonstrate that electron-electron interactions enhance the long-range pair-pair correlations for SC of d-wave symmetry preferentially at density 0.5. We further discuss the effect of lattice frustration on pairing and CO in this class of materials.

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