

Abstract Submitted
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What is special with molecular valence 3 in metal-intercalated phenacenes?¹ SUMITENDRA MAZUMDAR, TIRTHANKAR DUTTA, University of Arizona — Two important observations are pertinent to the newly discovered metal-intercalated polycyclic aromatic hydrocarbon (PAH) superconductors (examples include, phenanthrene, picene, coronene, and dibenzopentacene): (a) Why are the acenes with linearly fused benzene rings not superconducting? (b) Why does T_c in the PAHs peak only at metal doping ~ 3 ? In order to address these questions, we have developed a correlated-electron minimal model for phenanthrene ions in solid state, in the reduced space of the two lowest unoccupied molecular orbitals of neutral phenanthrene. Our model is general and can easily be extended to normal states of other PAHs, like, picene and coronene, although the computations would be more demanding. Exact many-body finite cluster calculations on phenanthrene show that while the systems with molecular charges of -1 and -2 are one- and two-band Mott-Hubbard semiconductors, respectively, molecular charge -3 gives two nearly $\frac{3}{4}$ -filled bands. The carrier density per active molecular orbital in the superconducting aromatics is nearly the same as that in the organic charge-transfer solids, and we believe that this common carrier density may be the key to understanding unconventional superconductivity in these molecular superconductors.

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