

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Crystal structure, electronic properties, and superconductivity mechanism of La-Phenanthrene¹ SHAHAB NAGHAVI, SISSA, CNR-IOM Democritos, MICHELE FABRIZIO, SISSA, ICTP, CNR-IOM Democritos, TAO QIN, SISSA, CNR-IOM Democritos, ERIO TOSATTI, SISSA, ICTP, CNR-IOM Democritos — Recently, polycyclic aromatic hydrocarbon (PAH) molecular solids: picene, coronene, dibenzopentacene, phenanthrene among them, have been reported to turn from insulating to metallic and superconducting upon intercalation of electron-donating atoms, such as K, Ba, La. Despite experimental uncertainties, understanding these novel light-element based superconductors is important since both electron phonon coupling and electron electron correlations seem important, as indicated by early theory work. Choosing La-Phenanthrene (La-PA) as our working case, we first search for the theoretical optimal crystal structure and electronic properties by first principles density functional calculations. We single out a stable insulating phase with $P1$ symmetry and, slightly higher in energy, a metastable metallic $P2_1$ phase—the same (higher) symmetry of pristine PA, also proposed for La-PA. A tight binding model representing the metallic La-PA electronic structure, its dominant electron phonon coupling with an intermolecular dimerizing mode, and an intramolecular Coulomb U is formulated and discussed. In that model it can be argued that BCS pairing may be essentially unhindered by the Coulomb repulsion. Being symmetry-based, the mechanism could apply to other PAH superconductors as well.

¹Supported by EU-Japan Project LEMSUPER

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Date submitted: 08 Nov 2012

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