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Electron correlations in C_{60} and aromatic superconductors

YUSUKE NOMURA, KAZUMA NAKAMURA, RYOTARO ARITA, Department of Applied Physics, University of Tokyo — Recent discovery of superconductivity in fcc/A15 Cs_3C_{60} under pressure and in aromatic compounds (ex. alkali-doped picene) has stimulated a renewed interest in molecular superconductors such as K_3C_{60} and Rb_3C_{60} . To clarify the mechanism of the superconductivity, it is essential to understand low-energy electronic structure of these systems. In the present study, we perform a systematic study for understanding the relation between electronic correlation and superconductivity in C_{60} and aromatic compounds [1]. We derived, from first principles, extended Hubbard models for twelve compounds: fcc K_3C_{60} , Rb_3C_{60} , Cs_3C_{60} (with three different lattice constants), A15 Cs_3C_{60} (with four different lattice constants), doped solid picene, coronene, and phenanthrene. We show that these compounds are strongly correlated and have similar energy scales of their bandwidths and interaction parameters. However, they have a different trend in the relation between the strength of the electronic correlation and superconducting-transition temperature. While the C_{60} compounds have a positive correlation, the aromatic compounds exhibit a negative correlation. [1] Y. Nomura, K. Nakamura, and R. Arita, Phys. Rev. B **85**, 155452 (2012).

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