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Dynamical Mean-Field Theory Study of Correlated Electronic Structures and the Phase Diagram of Hydrocarbon Superconductors MIN-JAE KIM, Department of Physics, Pohang University of Science and Technology, HONG CHUL CHOI, Department of Chemistry, Pohang University of Science and Technology, JI HOON SHIM, Department of Chemistry and Division of Advanced Nuclear Engineering, Pohang University of Science and Technology , B. I. MIN, Department of Physics, Pohang University of Science and Technology — We have studied correlated electronic structures and the phase diagram of electron-doped hydrocarbon molecular solids, based on the dynamical mean-field theory. We have determined the phase diagram of hydrocarbon molecular solids as functions of doping and energy parameters including the Coulomb correlation, the Hund coupling, and the molecular-orbital (MO) energy level splitting. We have found that the hydrocarbon superconductors (electron-doped picene and coronene) belong to the multi-band Fermi liquid state, while non-superconducting electron-doped pentacene belongs to the single-band state in the proximity of the metal-insulator transition. The size of the MO energy level splitting plays an important role in deriving the superconductivity of electron-doped hydrocarbon solids. The multi-band nature of hydrocarbon solids from the small MO energy level splitting boosts the superconductivity through the enhanced density of states at the Fermi level.

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