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Electronic structure and magnetic properties of the hydrocarbon K_3picene superconductor near the metal-insulator transition MINJAE KIM, B.I. MIN, Department of Physics, PCTP, Pohang University of Science and Technology, GEUNSIK LEE, HEE JAE KWON, Y.M. RHEE, JI HOON SHIM, Department of Chemistry, Pohang University of Science and Technology — Superconductivity has recently been observed in K-doped picene, K_3picene, which is a first organic superconductor in the hydrocarbon system with high transition temperature Tc=18K [1]. We have investigated the electronic structures and magnetic properties of K_3picene by density-functional theory. We have shown that the metal-insulator transition (MIT) is driven in K_3picene by 5% volume enhancement with a formation of local magnetic moment. Active bands for superconductivity near the Fermi level (E_F) are found to have hybridized character of LUMO and LUMO+1 picene molecular orbitals. Fermi surfaces of K_3picene manifest neither prominent nesting feature nor marked two-dimensional behavior. By estimating the ratio of the Coulomb interaction $U$and the band width $W$of the active bands near E_F , U/W, we have demonstrated that K_3picene is located in the vicinity of the Mott transition.

[1] R. Mitsuhashi *et. al.* Nature. 464, 76 (2010)

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