アルカリドープピセンをはじめとする
芳香族超伝導体の電子状態計算
Electronic Structure Calculations of Aromatic Superconductors: Alkali-doped Picene and Related Materials

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Solid picene has been recently reported to exhibit superconductivity under doping with alkali elements [1]. Their atomic configurations, however, have not been determined experimentally. In the present study, we systematically examined possible structures of $K_x$picene for x=1-4 allowing the lattice parameters and the atomic coordinates to be relaxed with no constraint [2]. For x=3, two of the obtained structures are shown in the figure below. While K_3picene contains all the potassium atoms in the molecular layer, K_2K_1picene contains the two potassium atoms in the layer and one between the layers. Although K_2K_1picene is higher in energy by 0.465 eV per molecule than K_3picene, it has lattice constants closer to the experimental values for x=2.9. The electronic structures near the Fermi level for all the obtained structures for x=0-4 were found to be well reproduced by LUMO- and LUMO+1-derived localized orbitals. Potassium-doped coronene is reported to be a superconductor as well [1]. We also discuss the commonalities and differences between the electronic structures of doped picene and coronene [3].

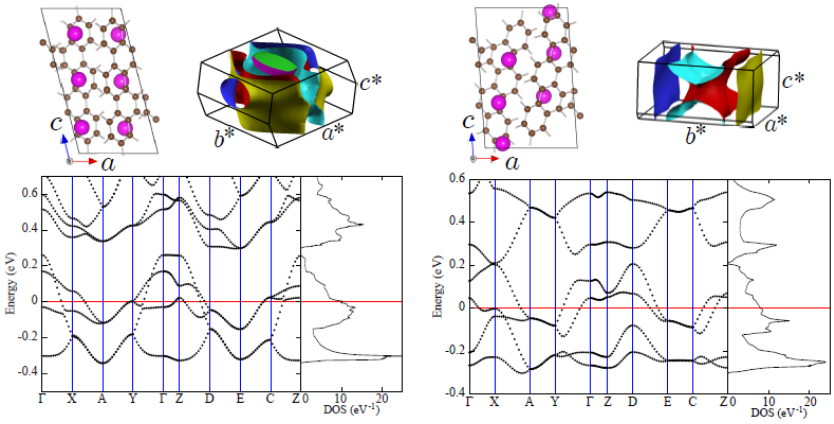

Fig. Geometries, band structures, and Fermi surfaces of K_3picene (left) and K_2K_1picene (right).

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