

Abstract Submitted
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Electronic structures of potassium-doped C_{60} encapsulated in BN nanotubes TAKASHI KORETSUNE, SUSUMU SAITO, Department of Physics, Tokyo Institute of Technology, JESSE NOFFSINGER, MARVIN L. COHEN, Department of Physics, University of California, Berkeley — Boron-nitride nanotubes have large band gap independent of chirality and are promising candidates for nanostructure control. Here, we investigate the electronic structure of potassium-doped C_{60} encapsulated in boron-nitride nanotubes using first-principles methods based on the density functional theory. We demonstrate that the material is one-dimensional metal where conducting electrons are only in the C_{60} chain. Interestingly, the material can have a large Fermi-level density of states, which indicates the possibility of various phase transitions including superconductivity as in the case of fcc K_3C_{60} . We therefore discuss the electron-phonon couplings as well as the pressure dependence of the electronic structures of this material.

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