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First principles study of cubane and alkali doped C60 solids
YOUNG-MOO BYUN, VINCENT CRESPI, Department of Physics, Penn State University — Alkali doped fullerene (C60) solids have been studied widely due to their interesting physical properties. Lately, an experimental group succeeded to dope cubane (C8H8) into the octahedral voids of faced-centered-cubic (FCC) C60 solids, demonstrating that not only atoms (and polyatomic cations), but also small neutral molecules can intercalated into C60 solids. We study the electronic properties of cubane-doped C60 solids using first-principles techniques and show that C60 solids doped with both cubane and alkali metals, in which alkali metals such as K and Rb occupy the tetrahedral voids are energetically favorable. Cubane molecules substantially dilate the C60 lattice, resulting in a very large density of states in a single-particle treatment and pronounced tendency towards electronic instability.

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