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Fermi surface changes in $LaFeAsO_{1-x}F_x$ using supercells, rigid band shifts, and the virtual crystal approximation[1] PAUL LARSON, University of Nebraska, SASHI SATPATHY, University of Missouri — There is currently great interest in the properties of the superconducting material LaFeAsO. While numerous calculations have been performed for this material, questions arise to which approximations describe the changes in the Fermi surface with doping. We have performed *ab initio* density functional studies of F-doping in the non-magnetic state using supercell calculations and compared these results to those obtained using rigid band shifts and the virtual crystal approximation (VCA). The Fermi surface consists mainly of Fe d and As p states with La and O states lying far from the Fermi level. Significant differences are found by comparing the supercell results with those of the rigid band shifts, but remarkable agreement is found for the Fermi surface using VCA calculations where the nuclear and electron charge are changed continuously to mimic the addition of electrons. P.Larson and S. Satpathy, condmat:arXiv 0810.4605v1.

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