

Abstract Submitted
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Theoretical visualization of atomic-scale impurity states in Fe-based superconductors¹ PEAYUSH CHOUBEY, PETER HIRSCHFELD, TOM BERLIJN, University of Florida, CHAO CAO, Hangzhou Normal University — We study the impurity induced local density of states (LDOS) in Fe-based superconductors, incorporating Wannier functions to obtain a higher resolution derived from a downfolding of density functional theory bands onto a 10-Fe tight-binding model. This enables us to compare our results with those obtained experimentally using STM. We solve the ten orbital Bogoliubov-de Gennes (BdG) equations for the single impurity problem and obtain the superconducting state lattice space Green's function, which is then transformed to the Wannier basis. The utility and limitations of this approximation are discussed.

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Peayush Choubey
University of Florida

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