

Two-dome superconductivity and Coulomb correlations in FeS

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Tetragonal FeS exhibits a puzzling “double-dome” superconducting phase diagram under pressure. To elucidate the microscopic origin of this phenomenon, we investigate the electronic structure evolution of FeS using a combination of Density Functional Theory and Dynamical Mean-Field Theory (DFT+DMFT). Unlike standard DFT, this approach explicitly treats dynamic electronic correlations, which are essential for accurately capturing the orbital-selective band renormalization in iron chalcogenides.

Our results demonstrate that electronic correlations play a crucial role in driving an electronic Lifshitz transition. The DMFT calculations provide a description of the Fe $3d_{z^2}$ orbital evolution, confirming that the sudden appearance of a hole pocket near the Γ point is responsible for the reemergence of superconductivity in the second dome. The inclusion of dynamic self-energy effects corrects the critical pressure of the transition compared to non-interacting models. Currently, calculations regarding the specific symmetry of the superconducting gap are in progress, utilizing the full interacting Green’s function to solve the linearized gap equation in the correlated regime.

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