First-principles theory of electron-spin fluctuation coupling and superconducting instabilities in iron selenide

JOHannes LIscHner, UC Berkeley and Lawrence Berkeley National Lab, TIMur BAZHIrov, UC Berkeley, Allan H. MAcDonald, UT Austin, Marvin L. COHEN, Steven G. LOUIE, UC Berkeley and Lawrence Berkeley National Lab — We present first-principles calculations of the coupling of quasiparticles to spin fluctuations in iron selenide and discuss which types of superconducting instabilities this coupling gives rise to. We find that strong antiferromagnetic stripe-phase spin fluctuations lead to large coupling constants for superconducting gaps with $s^{+/-}$ symmetry, but these coupling constants are significantly reduced by other spin fluctuations with small wave vectors. An accurate description of this competition and an inclusion of band structure and Stoner parameter renormalization effects lead to a value of the coupling constant for an $s^{+/-}$ symmetric gap which can produce a superconducting transition temperature consistent with experimental measurements.

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