

Abstract Submitted  
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**First-principle studies of electronic structure and magnetic excitations in FeSe monolayer**<sup>1</sup> TIMUR BAZHIROV, MARVIN L. COHEN, University of California, Berkeley — Recent experimental advances made it possible to study single-layered superconducting systems of iron-based compounds. The results show evidence of significant enhancement of superconducting properties compared to the bulk case. We use first-principle pseudopotential density functional theory techniques and the local spin-density approximation to study the electronic properties of an FeSe monolayer in different spin configurations. The results show that the experimental shape of the Fermi surface is best described by a checkerboard antiferromagnetic (AFM) spin arrangement. To explore the underlying pairing mechanism, we study the evolution of the non-magnetic to the AFM-ordered structures under constrained magnetization, and we estimate the electronic coupling to magnetic excitations involving transfer and increase of iron magnetic moments and compare it to the electron-phonon coupling. Finally, we simulate the substrate-induced interaction by using uniform charge doping and show that the latter can lead to an increase in the density of states at the Fermi level and possibly produce higher superconducting transition temperatures.

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