Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles theory of electron-spin fluctuation coupling and superconducting instabilities in iron selenide[1] 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.

[1]This work was supported by NSF Grant No. DMR10-1006184 and by DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the DOE at NERSC.

Johannes Lischner
UC Berkeley and Lawrence Berkeley National Lab

Date submitted: 14 Nov 2014 Electronic form version 1.4