Abstract Submitted
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Effect of Pressure on the Electronic Structure and Optical Properties of FeSe: A DFT+DMFT Study[1] SUBHASISH MANDAL, R.E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington, K. HAULE, Department of Physics and Astronomy, Rutgers University — Superconductivity in the iron-chalcogenide superconductors is extremely sensitive to pressure; T_c increases from 8 K to 37 K upon applying pressure[1]. In order to better understand the sensitivity of T_c to pressure in FeSe we have performed fully self-consistent Density Functional Theory - Dynamical Mean Field Theory (DMFT) (DFT-DMFT) computations with a continuous quantum Monte Carlo impurity solver as a function of compression and temperature. Using analytic continuation, we have computed spectral functions, Fermi surfaces, and the optical properties for comparison with experiments. Our preliminary results, obtained at room temperature show a $\sim 43\%$ reduction of the dc conductivity upon increasing the pressure from 0 to 2.6 GPa.

[1] S. Medvedev *et al.* Nat. Mater. **8**, 630 (2009).

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