Abstract Submitted
for the SES21 Meeting of
The American Physical Society

Monolayer FeSe deposited on $SrTiO_3$ ALEXANDER KELLERHOUSE, Francis Marion University, TOM BERLIJN, Oak Ridge National Lab, HUNTER SIMS , Francis Marion University — Monolayer FeSe deposited on $SrTiO_3$ exhibits a superconducting T_C of 40 – 80 K compared to 8 K in bulk FeSe. We have investigated how the electronic structure of FeSe depends on changes in the atomic structure of the substrate. To do this, we used density function theory (DFT) to simulate the atomic structure of FeSe on top of STO. We see that oxygen vacancies and the alignment of Se above the substate both affect the interlayer distance. With the altering of the interlayer distance doping of the compound is also affected. We also found that Ti impurities placed on the double-TiO layer further affected the bond lengths between FeSe and the surface below. The exact atomic structure of the FeSe/$SrTiO_3$ interface is difficult to determine from experimental data alone, and furthermore the real interface will inevitably be imperfect. We account for both this uncertainty and the likelihood of defects by implementing a Wannier-orbital-based approach that allows us to project the electronic structure, isolate the effect of impurities, and generate structures with arbitrary impurity concentrations. The resulting unfolded band structures are comparable to experimental ARPES spectra and may provide insight into how to isolate and replicate this enhances superconductivity in other materials.

Alexander Kellerhouse
Francis Marion University

Date submitted: 29 Sep 2021 Electronic form version 1.4