Combined ARPES and DFT+eDMFT investigation on high-temperature topological superconductivity in the $FeTe_xSe_{1-x}$ system

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So far, most of the studies of topological materials have focused on the single-particle regime where traditional band theory accurately reproduced experimental findings. A fundamentally unaddressed question is how strong electron-electron interactions drive a topological system far from the single-particle limit where electrons are close to being localized. Recently, the strongly correlated Fe(Te, Se) systems have been a point of interest in the literature as it is a potential system to exhibit high-temperature topological superconductivity. We use a combination of *ab initio* embedded dynamical mean-field theory (eDMFT), molecular beam epitaxial (MBE) growth, and time and angle-resolved-photoemission-spectroscopy (trARPES) to understand the correlated electronic structure and vibrational properties of the Fe(Te,Se) system under an applied in-plane strain. Using eDMFT, we compute structural parameters for various $FeTe_xSe_{1-x}$ systems including the chalcogen heights and the important A_{1g} phonon mode. In addition, we explore the effects of spin-orbit coupling and temperature to gain more insight into the topological phase transition, the nature of the hybridization, and the transition to the orbital-selective correlated phase. Computed eDMFT orbital-resolved spectral functions are found to be in excellent agreement with the ARPES data. Our combined ARPES + eDMFT approach unravels an interesting phase diagram of the Fe(Te, Se) system between superconductivity and topological non-trivial phase as a function of increasing electron correlation.