Competing instabilities at paraelectric/superconducting interfaces

The discovery of the new class of iron based high-Tc superconductors in 2008 lead to an enormous increase of research in this field of solid state physics. In particular the origin of the superconductor pairing mechanism is of high interest, since its identification may allow the designing new superconductors. In order to assist the clarification of this question we follow recent experiments of ultrathin FeSe films on SrTiO$_3$ to investigate from first principles the influence of strain and interface effects on the electronic structure of FeSe. First we compare our calculated electronic properties of coherent FeSe films under different tensile strains, corresponding to SrTiO$_3$ and MgO substrates, and electron/hole doping with experimental findings. The main result is that for moderate applied strain the spin density wave in FeSe is suppressed, whereas there is a sudden strong enhancement for larger strain. Given that superconductivity disappears in highly strained FeSe on MgO, our results thus give an interesting insight in which energy range the SDW still compete with superconductivity. The results of the comparison are further discussed with respect to the possibility of phonon pumping superconductivity in FeSe. In the last part we discuss the FeSe/STO superlattice, focusing on the competition of lattice and magnetic instabilities. The results are then discussed with respect to the conclusions made for coherent films. Finally we argue how only the interface termination of FeSe/SrTiO$_3$ superlattice determines the possibility of superconductivity within this system.

1. Kamihara, Y., Watanabe, T., Hirano, M. & Hosono, H. Iron-Based Layered Superconductor La[O$_{1-x}$F$_x$]FeAs (x= 0.05−0.12) with Tc= 26 K. Journal of the American Chemical Society 130, 3296–3297 (2008).