MAR15-2014-020295

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

First-principles study of the electron/spin-phonon interaction in compressed FeSe crystal and FeSe/STO system[1]

ZHONG-YI LU, Department of Physics, Renmin University of China

By using the first-principles calculations with van der Waals corrections, we have studied the electronic structures, lattice dynamics, and magnetic properties of crystal FeSe under hydrostatic pressure [1] and FeSe/STO system [2,3]. For bulk FeSe, the frequencies of all optical phonon modes increase with pressure. In a range between 5 and 6 GPa, the frequency of the A_{1g} mode, which relates to the Se height from the Fe-Fe plane, shows a sudden jump. This is also the pressure range within which the highest superconducting transition temperature Tc of FeSe is reached in experiments. In comparison with the other phonon modes, the zero-point atomic displacement of the A_{1g} mode also induces the strongest variation of local magnetic moment on Fe, which reaches the maximum around 5 GPa. These results suggest that the effect of phonon via spin-phonon coupling could not be omitted. For monolayer FeSe epitaxial film on $SrTiO_3$, the combined effect of electron doping and phonon readily leads to magnetic frustration between the collinear antiferromagnetic state and checkerboard antiferromagnetic Neel state. For bilayer FeSe epitaxial film on $SrTiO_3$, such a magnetic frustration is much easier induced by electron doping in its bottom layer than its top layer. The underlying physics is that the doped electrons are accumulated at the interface between the FeSe layers and the substrate. These results are consistent with the existing experimental studies.
[1] Q.-Q. Ye, K. Liu, and Z.-Y. Lu, Influence of spin-phonon coupling on antiferromagnetic spin fluctuations in FeSe under pressure: First-principles calculations with van derWaals corrections. Phys. Rev. B **88**, 205130 (2013). [2] K. Liu, Z.-Y. Lu, and T. Xiang, Atomic and electronic structures of FeSe monolayer and bilayer thin films on SrTiO3 (001):First-principles study. Phys. Rev. B **85**, 235123 (2012). [3] K. Liu, B.-J.Zhang, and Z.-Y. Lu, First-principles study of magnetic frustration in FeSe epitaxial films on SrTiO3. Submitted.

[1]Work supported by National Natural Science Foundation of China (Grants No. 11004243 and No. 11190024), National Program for Basic Research of MOST of China (Grant No. 2011CBA00112).