Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Oxygen vacancy induced flat phonon mode at FeSe/STO interface. YUN XIE, HAI-YUAN CAO, YANG ZHOU, Fudan Univ, SHIYOU CHEN, East China Normal University, HONGJUN XIANG, XINGAO GONG, Fudan Univ, FUDAN UNIVERSITY TEAM — A high-frequency optical phonon mode of SrTiO3(STO) was found to assist the high-temperature superconductivity observed recently at the interface between monolayer FeSe and STO substrate. However, the origin of this mode is not clear. Through first-principles calculations, we find that there is a novel polar phonon mode on the surface layers of the STO substrate, which does not exist in the STO crystals. The oxygen vacancies near the FeSe/STO interface drives the dispersion of this phonon mode to be flat and lowers its energy, whereas the charge transfer between STO substrate and FeSe monolayer further reduces its energy to 81 meV. This energy is in good agreement with the experimental value fitted by Lee et al. for the phonon mode responsible for the observed replica band separations and the increased superconducting gap. The oxygen-vacancy-induced flat and polar phonon mode provides clues for understanding the origin of high Tc superconductivity at the FeSe/ STO interface.

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Date submitted: 03 Dec 2015 Electronic form version 1.4