Abstract Submitted
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Electronic structure and lattice dynamics at the interface of single layer FeSe and $SrTiO_3$[1] TOWFIQ AHMED, Los Alamos Natl Laboratory, ALEXANDER BALATSKY, Los Alamos Natl Lab and Nordita, JIAN-XIN ZHU, Los Alamos National Laboratory — Recent discovery of high-temperature superconductivity with the superconducting energy gap opening at temperatures close to or above the liquid nitrogen boiling point in the single-layer FeSe grown on $SrTiO_3$ has attracted significant interest. It suggests that the interface effects can be utilized to enhance the superconductivity. It has been shown recently that the coupling between the electrons in FeSe and vibrational modes at the interface play an important role. Here we report on a detailed study of electronic structure and lattice dynamics in the single-layer FeSe/$SrTiO_3$ interface by using the state-of-art electronic structure method within the density functional theory. The nature of the vibrational modes at the interface and their coupling to the electronic degrees of freedom are analyzed. In addition, the effect of hole and electron doping in $SrTiO_3$ on the electron-mode coupling strength is also considered. [1] Q. Y. Wang et al., Chin. Phys. Lett. 29, 037402 (2012); [2] Jian-Feng Ge et al., Nature Mater. 14, 285 (2014).

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