清华大学高等研究院

Institute for Advanced Study, Tsinghua University

学术报告

Title: **Electronic structure of FeSe thin films: a first-principles study**

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Time: **2:00pm, Oct 16 (Friday), 2015**

Venue: **Conference Hall 322, Science Building, Tsinghua University**

Abstract

Based on the density functional theory, we have systematically studied FeSe monolayer on TiO2 terminated SrTIO3 (001) surface. It is revealed that the striking disappearance of the Fermi surface around the Brillouin zone center can be well explained by the antiferromatnetic (AFM) phase. A tight-binding model Hamiltonian is proposed to describe the main features. We have in addition studied potassium-adsorbed FeSe/SrTiO3 with different K coverage. A first-principles band unfolding algorithm is developed to reconstruct the electronic band structure in the FeSe primitive cell representation. We explain the Fermi surface topology observed in experiment and formulate the amount of doped electrons as a function of atomic K coverage. These results indicate that charge transfer across the interface and the associated electric field play an important role in shaping the band structure as observed in experiment. In particular, with an experimentally accessible electron doping concentration (> 0.2 e per FeSe formula unit), an electron-like Fermi pocket will emerge at Γ point, which should manifest itself in modulating the high-temperature superconductivity of FeSe thin films.