

**Stony Brook University
The Graduate School**

Doctoral Defense Announcement

Abstract

Translational Symmetry Breaking in Materials:

First-principles Wannier Function Study

By

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The spatial periodicity of the crystal structure dictates the electronic band structure theory as the fundamental paradigm in solid state physics. The original translation in materials is commonly broken with an enlarged unit cell required by the spontaneously developed long-range order or multiple competing periodicities. The former happens in the systems undergoing the phase transition to antiferromagnetism, charge/spin density waves or lattice distortion. The latter is originated from the intrinsic arrangement of the multiple atom system or the externally introduced impurities. The emergence of broken symmetry can significantly modify the electronic structure, shift the chemical potential, and change the electric, magnetic or optical response in the experimental measurement.

In this thesis, the impact of translational symmetry breaking on various materials is investigated by utilizing the First-principles Wannier functions. We represent the electronic structure by calculating the one-particle spectral function in the reference momentum basis corresponding to a shorter periodicity. In the first case, the lattice distortion in Li metal at high pressures is found to cause the Fermi surface topological change, termed Lifshitz transition. We identify this transition triggers an anomalous enhancement of superconductivity. In the second case, we formulate a simple way to create massless Dirac particles in any effective one-band two-dimensional lattice from the inspiration of understanding Dirac cone formation in graphene. In the last case, we would discuss the staggered tetrahedral structure in Fe-based superconductors can imply the orbital-parity selective physics in the quasi-particles and superconducting pairing.

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