Stony Brook University
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Doctoral Defense Announcement

Abstract

Effects of Disordered Dopants on The Electronic Structure of Functional Materials:

Wannier Function-Based First Principles Methods for Disordered Systems

By

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Doping is one of the most powerful tools for tuning the electronic properties of functional materials. Well known examples include doped semiconductors and the Cu and Fe based high temperature super conductors. Besides introducing charge carriers and chemical pressure, it is almost inevitable that dopants will introduce quenched disorder into the system. This can have a wide range of consequences for the electronic structure, such as electric and thermal resistance, a deformation of the nodal structure of a super conductor or Anderson localization.

In this thesis the influence of disordered dopants is studied by calculating the configuration-averaged spectral function <A(k,w)> from first principles within the super cell approximation. To overcome two major problems of the super cell approximation, the band folding and the computational expense, two Wannier function based first principles techniques are developed.

The developed methodology is applied to address two realistic materials problems. The first problem being on the influence of disorder on the Fermi surface of NaxCoO2, an important thermoelectric material. The second problem is on the role of oxygen vacancies in the room temperature ferromagnetism in the recently discovered dilute magnetic semiconductor Cu:ZnO.

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