



北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Weekly Seminar

Electronic Correlation, Magnetism and Superconductivity in Iron Pnictides and Chalcogenides: A Dynamical Mean Field Theory Perspective.

Zhiping Yin

Rutgers University

Time: 4:00pm, April. 8, 2015 (Wednesday)

时间: 2015年4月8日 (周三) 下午4:00

Venue: Room W563, Physics Building, Peking University

地点: 物理楼 西563

Abstract

Electronic correlation has profound impacts on many properties of correlated materials, such as electron-phonon coupling, magnetism and superconductivity. However, strongly correlated materials have long resisted first-principles modeling due to their complexity arising from non-perturbative strength of the interaction. The Dynamical Mean Field Theory in combination with the Density Functional Theory has recently changed this position, and enabled detailed modeling of the electronic structure of complex heavy fermions, transition metal oxides, chalcogenides and arsenides. The recently discovered iron-based superconductors are a new class of strongly correlated materials, coined Hund's metals. In the paramagnetic state, the Hund's rule coupling J leads to a large fluctuating local moment on the iron atom, substantially enhanced mass of the low-energy quasiparticles, and a low coherent temperature. The quasiparticles at intermediate temperature and intermediate energy scale show strong deviations from the Fermi liquid theory with a significant transfer of spectral weight from low to high energies. The first-principles simulations with the Dynamical Mean Field Theory combined with Density Functional Theory not only uncover the origin of these anomalous properties, but also successfully explains the key properties of these material: such as the mass renormalizations and anisotropy of quasiparticles, the crossover into an incoherent regime above a low temperature scale, and the magnetic excitations in energy and momentum space. The first-principles simulations of the two particle vertex function allows us to study the spin dynamics and superconducting pairing symmetry in a large number of iron-based superconductors where a novel orbital-antiphase $S_{\pm}$ pairing symmetry was uncovered recently which may be realized in LiFeAs , optimal doped $(\text{Ba,K})\text{Fe}_2\text{As}_2$ and other iron superconductors.

About the Speaker

Dr. Zhiping Yin obtained his B.S. in physics from Peking University in 2005 and his Ph.D in physics from University of California Davis in 2009. He is currently a research associate at Rutgers University working with Prof. Gabriel Kotliar. His research area has been theoretical and computational condensed matter and material physics with an emphasis on strongly correlated electron systems and high temperature superconductivity, in which he has made a number of important contributions. For example, he has established the mechanism of electronic correlation driven strong electron-phonon coupling mediated superconductivity and solved a thirty-year old puzzle in the bismuthates and chloronitrides. He defines the notions of Hund's metals and Hund's insulators which have distinct physics from conventional Mott-Hubbard insulators. He found a simple form of superconducting pairing in the orbital space and uncovered a novel orbital-antiphase pairing state for the iron-based superconductors which naturally explains a number of experimental observations. He has published a number of research papers in leading scientific journals including Nature Physics, Nature Materials, Nature Communications, Physics Review X, Physics Review Letters, and PNAS. His latest research interest is rational design of complex functional materials by combining theory, computation and experiment. He has successfully designed a new class of mixed-valent thallium halide materials which are promising candidates for high temperature superconductivity.