TECHNISCHE UNIVERSITÄT WIEN
Vienna | Austria

INSTITUT FÜR FESTKÖRPERPHYSIK
Institute of Solid State Physics

Wiedner Hauptstr. 8-10/138, 1040 Wien
www.ifp.tuwien.ac.at

EINLADUNG zum IFP-SEMINAR

Fermi Arc Evolution and Doping Mechanism in High-Temperature Superconductors

Denis Sunko

Department of Physics, Faculty of Science, University of Zagreb, Croatia

Host:	Neven Barišić
Termin:	Wednesday, 9. November 2016, 16:00 Uhr
Ort:	Institut für Festkörperphysik, TU Wien
	Wiedner Hauptstraβe 8-10, 1040 Wien
	Seminarraum DC rot 07 (roter Bereich, 7. OG)
Förderer:	FWF P27980-N36 ARCS

Two distinct lines of research in the high-temperature cuprates are brought together by considering the atomic orbitals involved in the metallicity of the underdoped compounds.

First, realistic Fermi surface (FS) evolution of $La_{2-x}Sr_xCuO_4$ (LSCO) with Sr doping is obtained within an extensive ab-initio framework including advanced band-unfolding techniques. Ordinary Kohn-Sham DFT+U can reproduce the observed metal-insulator transition and arc growth, when not restricted to the paramagnetic solution space. Both arc protection and the inadequacy of the rigid-band picture are consequences of a rapid change in orbital symmetry at the Fermi energy: the material undergoes a dimensional crossover along the Fermi surface, between the nodal (2D) and antinodal (3D) regions.

The same calculation shows that the Sr hole stays localized in the vicinity of the dopand atom, indicating that metallization of the Cu-O plane is due to an orbital transition between Cu and O planar sites, originally proposed by Mazumdar in 1989. We can directly observe effects of the transition in charge transfers among in-plane atoms, which are different than predicted by non-interacting coherent models. This "ionic doping" mechanism connects the physical and chemical meanings of the chemical potential.

Second, the orbital transition is experimentally confirmed by replacing 3% (molar) of Cu in nearly optimally doped $YBa_2Cu_3O_{6.92}$ powder with isotopically pure ^{67}Zn, lowering T_c to 57 K. The pure nuclear quadrupole resonance (NQR) spectrum of ^{67}Zn, measured for the first time, shows that each Zn dopand surrounds itself with an insulating cluster, reverting the orbital transition locally back towards the parent-compound configuration. An unexpected asymmetry of the NQR signal is traced to the same splitting of the planar oxygens as the LTT tilt in LSCO, also well known to strongly lower T_c. This elevates the absence of intra-unit-cell oxygen-oxygen energy splitting to a universal requirement for superconductivity in the cuprates, providing a microscopic insight into the superconducting mechanism.