Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Fermi Arc Evolution and Doping Mechanism in High-Temperature Superconductors DENIS K. SUNKO, DAMJAN PELC, MIROSLAV POŽEK, VITO DESPOJA, Department of Physics, Faculty of Science, University of Zagreb, Bijenička cesta 32, HR-10000 Zagreb, Croatia, PREDRAG LAZIC, Theoretical Physics Division, Rudjer Boskovic Institute — We calculate realistic Fermi surface (FS) evolution of $La_{2-x}Sr_xCuO_4$ (LSCO) with Sr doping within an extensive ab-initio framework including advanced band-unfolding techniques. We show that ordinary Kohn-Sham DFT+U can reproduce the observed metal-insulator transition and arc growth, when not restricted to the paramagnetic solution space. We elucidate both arc protection and the inadequacy of the rigid-band picture as 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. In LSCO, this crossover accounts for FS arcs and the antinodal pseudogap, otherwise ubiquitous phenomena in high-Tc cuprates. The orbital transition is experimentally confirmed by replacing 4% of planar Cu in nearly optimally doped $YBa_2Cu_{2.97}Zn_{0.03}O_{6.92}$ powder with ^{67}Zn isotope, lowering T_c to 57 K. The NQR spectrum of ^{67}Zn, measured for the first time, shows that each Zn dopand surrounds itself with an insulating cluster. Zn destroys the SC metal by a Coulomb "domino effect" which reverts the orbital transition locally and pushes a significant number of surrounding sites back towards the parent-compound configuration.

Predrag Lazic
Rugjer Boskovic Inst

Date submitted: 13 Nov 2014 Electronic form version 1.4