Electron Glass Phase with Resilient Zhang-Rice Singlets in $LiCu_3O_3$

Armando Consiglio[1,2], Gianmarco Gatti[3,4], Edoardo Martino[3], Tobias Hofmann[1], Ronny Thomale[1], Giorgio Sangiovanni[1], Domenico Di Sante[5], Martin Greiter[1], Marco Grioni[3], Simon Moser[3,6,7], et al.

1. Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

2. Istituto Officina dei Materiali, Consiglio Nazionale delle Ricerche, Trieste I-34149, Italy

3. Institute of Physics, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

4. Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest-Ansermet, 1211 Geneva, Switzerland

5. Department of Physics and Astronomy, University of Bologna, Bologna, Italy

6. Advanced Light Source (ALS), Berkeley, California 94720, USA

7. Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg 97074, Germany

Abstract: This study highlights that in the antiferromagnetic cuprate $LiCu_3O_3$, despite extensive Lithium substitutional disorder, the Zhang-Rice singlets remain largely unaffected by impurity scattering, and the system exhibits a Lithium-induced electron glass behavior in charge transport.

$LiCu_3O_3$ is an antiferromagnetic cuprate where Lithium substitution disrupts the native arrangement of edge-sharing Cu(II)O and Cu(I) ions. Using angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT), we identify two distinct insulating electronic subsystems induced by Lithium substitutional disorder. The first subsystem features a Cu d_{z2}/O$_{pz}$ valence band dispersing on the Cu(I) plane, while the second subsystem reveals a robust Cu $3d_{x2-y2}$/O $2p_{x,y}$ derived Zhang-Rice singlet (ZRS) band on the Cu(II)O planes. Li substitution stabilizes the insulating ground state and induces a unique 2D electron glass behavior in charge transport, as observed through ARPES. Our study [1] identifies the presence of ZRS in a cuprate-based electron glass and demonstrates the resilience of ZRS quasiparticles due to quantum entanglement. These findings could have significant implications not only for advancing the understanding of cuprate superconductors but also for the development of future technologies reliant on quantum coherence. Specifically, the ability to stabilize quantum states against external disturbances through quantum entanglement may be crucial for the realization of quantum computers.

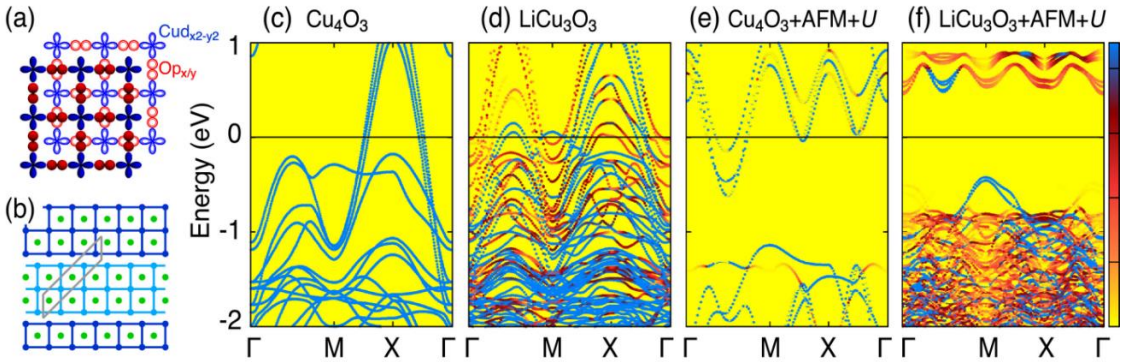

Fig. 1. (a) Decomposition of the CuO plane into two corner-sharing CuO_2 sublattices. (b) Most energetically favorable periodic ordering motif of a cuprate plane with 40% Li substitution. Light and dark blue squares represent Cu(II)O_2 plaquettes on different sublattices and green dots represent Li ions. (c-f) Electronic band structure of $LiCu_3O_3$ obtained considering different system's features. AFM refers to the antiferromagnetic arrangement, and *U* indicates the inclusion of a Hubbard term on the Cu sites.

References

[1] A. Consiglio, G. Gatti, E. Martino, L. Moreschini, J. C. Johannsen, K. Prša, P. G. Freeman, D. Sheptyakov, H. M. Rønnow, R. Scopelliti, A. Magrez, L. Forró, C. Schmitt, V. Jovic, C. Jozwiak, A. Bostwick, E. Rotenberg, T. Hofmann, R. Thomale, G. Sangiovanni, D. Di Sante, M. Greiter, M. Grioni, and S. Moser, "Electron glass phase with resilient Zhang-Rice singlets in LiCuO3O3," Phys. Rev. Lett. 132, 126502 (2024). https://doi.org/10.1103/PhysRevLett.132.126502