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Mott-Hubbard excitons in edge-sharing CuO4 chains

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Compounds composed of chains of edge sharing Cu2+O4 plaquettes have the peculiar property that the magnitude of the nearest-neighbor hopping matrix element along the chains is anomalously small due to the orthogonality of the 2pσ orbitals on oxygen ions adjacent to the Cu ion. By virtue of their exceptionally narrow electronic bandwidths, these compounds provide a highly favorable platform for the investigation of exciton formation and the interplay between spin and charge correlations in cuprates. We have performed a comprehensive ellipsometric study of the charge excitations across the optical gap in high-quality LiCuVO4 [1], NaCu2O2 [2], Li2CuO2, CuGeO3 and α-CuV2O6 single crystals. In all these compounds, the excitonic states associated with the Zhang-Rice singlet state were assigned. For photon polarization along the chains, the data reveal a weak but well-resolved two-peak structure forming the absorption edge whose spectral weight is strongly enhanced upon cooling near the magnetic ordering temperature. These bands were identified as exciton doublets, originating from the long-range Coulomb interaction between the nearest and the next-nearest-neighbour Cu sites along the chains. These results have not only persuasively demonstrated the formation of the Mott-Hubbard excitons, but also quantified characteristic energy scales, such as the local Hubbard U (2.55 – 4.3 eV) and long-range Coulomb V (0.8 – 1.6 eV) interactions.

[1] Y. Matiks, P. Horsch, R. K. Kremer, B. Keimer, A. V. Boris, Phys. Rev. Lett. 103, 187401 (2009)
[2] Y. Matiks, A. N. Yaresko, K. Myung-Whun, A. Maljuk, P. Horsch, B. Keimer, A. V. Boris, Phys. Rev. B 84, 245116 (2011)

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