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Computational Studies of Realistic Multiband Models of the Copper Oxides

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High temperature superconductivity was achieved by introducing holes in a parent compound consisting of copper oxide layers separated by spacer layers. It is possible to dope some of the parent compounds with electrons, and their physical properties are bearing some similarities but also significant differences from the hole doped counterparts. Here, we use a modern first principles method, to study the electron doped cuprates and elucidate the deep physical reasons why their behavior is so different than the hole doped materials. We find that electron doped compounds are Slater insulators, e.g. a material where the insulating behavior is the result of the presence of magnetic long range order. This is in sharp contrast with the hole doped materials, where the parent compound is a Mott charge transfer insulator, namely a material which is insulating due to the strong electronic correlations but not due to the magnetic order. In particular, we point out that both hole and electron doped compounds are located close to the charge-transfer insulator to metal transition, and we discuss the consequences for optical and specific heat measurements done for the normal state, and additional consequences for the magnetic and superconducting orders of electron and hole doped copper oxides.

Work done in collaboration with Kristjan Haule and Gabriel Kotliar, Rutgers University.