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Pressure induced hole charge transfer in Sr_2IrO_4

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As opposed to the Mott-insulating ground state found in the 3d-electron compounds, a metallic ground state is expected to be found in Ir based TMOs, due to the extended 5d electronic orbitals of the Ir ions. However, the n=1 member of the Ruddlesden-Popper perovskite family $Sr_{1+n}Ir_nO_{3n+1}$, Sr_2IrO_4, shows a non metallic behavior[1]. Its insulating ground state arises from the cooperative effect of the onsite Coulomb repulsion and strong spin orbit coupling, leading to a Jeff=1/2 Mott-insulating ground state [2].

A metallic state can be induced in Sr_2IrO_4 by electron or hole doping [3]. Another way to raise conductivity and to overcome the charge repulsion is to increase the electronic bandwidth with respect to the on-site Coulomb repulsion, which can be done by applying hydrostatic pressure[4]. However Sr_2IrO_4 shows a persistent insulating behavior under applied hydrostatic pressure[5-7]. While it has been suggested that the absence of metallization with pressure may come from an unexpected robustness of the lattice[6], more recent studies under pressures suggested a peculiar lattice dynamics with pressure preventing an efficient bandwidth renormalization, required to overcome the onsite Coulomb repulsion[7].

In order to investigate the evolution of the electronic structure of Sr2IrO4 under applied hydrostatic pressure, we performed infrared optical spectroscopy measurements under pressure. Optical conductivity analysis provides evidences for a Mott gap renormalization associated with in-gap state formation with pressure. These in-gap states originate mainly from a fillling control mechanism, arising from pressure induced hole doping of the IrO_2 planes due to high order lattice anisotropy corrections to the cubic crystal field characteristic of 5d electron systems[8,9]. However, despite the presence of in-gap states, the system remains highly incoherent in the investigated pressure range, as revealed by transport measurements. Also, a novel excitation develops withpressure. Its energy scale and its pressure evolution clearly indicates that lattice, charge and magnetic correlations remain highly intricated at high pressure.

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