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Polaronic hole-trapping in doped insulating oxide CESARE FRANCHINI, GEORG KRESSE, RAIMUND PODLOUCKY, University of Vienna — In transition-metal oxides, local electronic correlation effects dominate the physics, and lattice degrees of freedom are often only treated as external perturbations. However, in systems dominated by s and p electrons, electronic correlation is expected to be less important, and in agreement with this conjecture, we show that lattice degrees of freedom are crucial to account for the hole doping driven insulator-to-metal/superconducting transition (IMT) in $Ba_{1-x}K_xBiO_3$. Specifically, by using hybrid-DFT we show that Bi^{3+} sites trap two holes from the valence band accompanied by a large local lattice distortion, commonly referred to as bipolaronic state. We show that in pure $BaBiO_3$ a single peak in the imaginary part of the dielectric function is visible which corresponds to the charge-ordered excitation between Bi^{3+} and Bi^{5+} sub-bands. Upon hole-doping a second peak emerges at $x = 0.125$ connected with the bipolaronic excitation. At $x = 0.25$ the bipolaronic peak increases in intensity and is shifted towards lower energy, thus indicating the incipient IMT observed at $x \approx 0.3$. Our results describe all relevant experimental results.

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