Chiral Plaquette Polarons and the Universal Thermopower of Cuprate Superconductors

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UB3LYP ab-initio band structure calculations on the high temperature cuprate superconductor La$_{2-x}$Sr$_x$CuO$_4$ find two types of doped holes. The lowest energy state is the apical polaron where the hole is formed in the out-of-plane O pz nearest the Sr dopant. At an energy 0.06 eV higher, a plaquette polaron is stabilized consisting of an out-of-plane hole localized on the four-site Cu plaquette nearest the Sr atom. It is known that the cuprates have a “universal” room-temperature thermopower that is a function only of the hole doping in the CuO$_2$ planes. We show that this observation is a consequence of plaquette polarons and their percolation.