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The Impact of an Oxygen Dopant in an ideal $Bi_2Sr_2CaCu_2O_{8+\delta}$ Crystal STEVE JOHNSTON, University of Waterloo, Waterloo, ON, Canada., FRANCOIS VERNAY, Paul Scherrer Institut, Villigen PSI, Switzerland, T. P. DEVEREAUX, SLAC National Lab, Stanford, Menlo Park, CA — Scanning tunneling microscopy studies have shown that local nanoscale pairing inhomogeneities are correlated with interstitial oxygen dopants in $Bi_2Sr_2CaCu_2O_{8+\delta}$. Combining electrostatic and cluster calculations, we examine the impact of a dopant on the local Madelung and charge transfer energies, magnetic exchange J , Zhang-Rice mobility, and interactions with the lattice. It is found that electrostatic modifications locally increases the charge transfer energy and slightly suppresses J. It is further shown that coupling to c-axis phonons is strongly modified near the dopant. The combined e?ects yield broadened spectral features, reduced charge gap energies, and a sizable local increase of J implying a strong local interplay between antiferromagnetism, polarons, and superconducting pairing.

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