Energy-lowering structural distortions in cuprates: impact on crystal and electronic structures

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A comprehensive description of cuprates is particularly challenging due to the interplay of strong electronic interactions and complex crystal structures. While strong electronic correlations can be captured by many-body methods such as density matrix renormalization group (DMRG) and quantum Monte Carlo (QMC), prior works often utilize idealized Hamiltonians that dismiss structural complexities [1-2]. However, realistic structural distortions can lead to significant effects such as symmetry breaking and spatial variations in superconducting gaps [3-4] which are not captured in simplified models.

Reliable structure predictions can be provided by first-principle calculations. We apply density functional theory (DFT) to provide a realistic description of the normal state of the cuprate Bi-2212 ($Bi_2Sr_2CaCu_2O_{8+x}$), focusing on its structural, electronic, and magnetic properties. Our approach emphasizes the crucial role of structural distortions that lower the energy of the system, allowing us to: (a) accurately describe the experimentally observed insulating antiferromagnetic (AFM) ground state of the undoped parent compound (in contrast to the metallic state predicted by previous *ab initio* studies); (b) identify numerous low-energy competing spin and charge stripe orders in the hole-overdoped (x=0.25) material that are nearly degenerate in energy with the AFM ordered state, indicating strong spin and charge fluctuations; (c) predict the lowest-energy hole-doped x=0.25 crystal structure that exhibits long-range structural distortions and whose predicted oxygen dopant positions match high-resolution scanning transmission electron microscopy (STEM) measurements; and (d) describe electronic bands near the Fermi energy with flat antinodal dispersions and Fermi surfaces that in agreement with angle-resolved photoemission spectroscopy (ARPES) measurements and provide a clear explanation for the structural origins of the so-called ``shadow bands".

Through these findings, we demonstrate how critical the inclusion of realistic structural details is for the accurate modeling of complex materials such as Bi-2212, paving the way for more accurate many-body studies and a deeper understanding of the superconducting properties.

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References

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