New Generation of First-Principles Modeling of Cuprates

Scientific Achievement

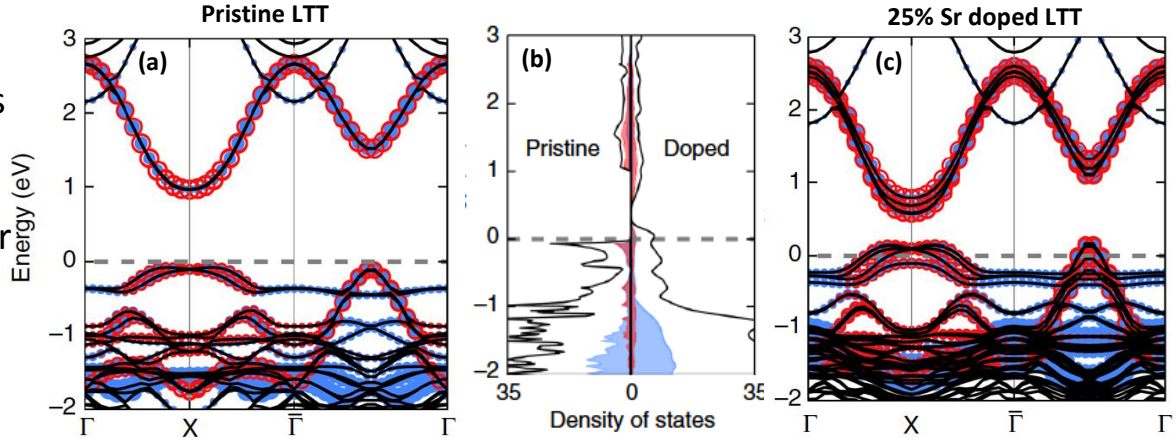
An accurate first-principles description of the electronic structure of $La_{2-x}Sr_xCuO_4$ high-T_c compound is obtained, without using any free parameters (no Hubbard U invoked).

Significance and Impact

Opens a pathway for a new generation of studies of cuprates and other correlated materials long considered to lie beyond the scope of the density functional theory.

Research Details

- The recent SCAN density functional is shown to yield the correct insulating ground state of La_2CuO_4 and its transition to the metallic state with Sr doping. All other density functionals fail in this regard.
- Theoretically predicted anti-ferromagnetic state of La_2CuO_4 reproduces experimental band gap, value and alignment of Cu moment in the cuprate plane, and value of the magnetic exchange coupking.



Electronic structure of pristine and 25% Sr doped low-temperature tetragonal (LTT) phase of La_2CuO_4 (LCO): (a) Insulating band structure of pristine anti-ferromagnetic LCO. (b) Densities of states of pristine and doped LCO are compared. (c) Metallic band structure of 25% Sr doped LCO. Orbital characters are shown for oxygen p_x+p_y (blue, filled circles) and copper d_{x2-y2}, pointing along the O-Cu-O bond, (red, empty circles), with marker size indicating strength of the projection.

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Work was performed at Northeastern and Tulane Universities