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Model Constraction and Fluctuation Exchange Study of a New Cuprate Superconductor $Ba_2CuO_{3+\delta}$

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Despite a long history exceeding three decades, the high-T_c cuprate superconductors have basically the same essential ingredient, the CuO_2 plane. Typically, high-T_c cuprates have a layered perovskite structure, where the Cu-O octahedron is elongated along the c axis, so that the $3dx^2$-y^2 orbital is located at the top among the $3d$ bands. In a previous study[1], it was shown that the separation of the $3dx^2$-y^2 orbital from other (especially $3d3z^2$-r^2) orbitals plays an important role in realizing high T_c d-wave superconductivity. Therefore, a large apical O height should in general favor high T_c as far as the CuO_2 plane is concerned with about 15% hole doping being "optimal" for the highest T_c.

Recently, Li *et al.* [2] reported high-T_c superconductivity in a new cuprate $Ba_2CuO_{3+\delta}$ with a K_2NiF_4-like layered structure. There, they find several unique features which strongly suggest that the material is a different type of cuprate superconductor that opens up a new paradigm. Namely, a large amount of O vacancies are present within the CuO_2 planes, and a great amount of holes are doped which should cause a large deviation of the Cu valence from 2+. Also, the distance between Cu and the apical O is shorter than the in-plane Cu-O distance, so that the octahedron is compressed along the c axis. This should result in a crystal field where the $3d3z^2$-r^2 orbital is lifted in energy above the $3dx^2$-y^2 orbital. These findings suggest that the mechanism of superconductivity in the $Ba_2CuO_{3+\delta}$ may be considerably different from that for the conventional cuprates.

For the 2-1-3 composition in particular, the chain structure is known to be stable in an actual material Sr_2CuO_3. As another possibility within the 2-1-3 composition, here we consider a Lieb lattice type structure. First principles total-energy calculation performed with the VASP code shows that the chain and the Lieb lattice structures are close in the total energy, so that the latter may also be considered as a candidate. Focusing on these two structures, we construct multiorbital Hubbard models, and discuss the possibility of superconductivity within the fluctuation exchange approximation.

[1] H. Sakakibara *et al.*, Phys. Rev. B **89**, 224505 (2014).
[2] W. M. Li *et al.*, Proc. Natl. Acad. Sci. U.S.A. **116**, 12156 (2019).

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