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Support information

Predicting Multiple Dirac-cones and Ultrahigh Fermi Velocity in Perovskite R-3c Phase $LaCuO_3$

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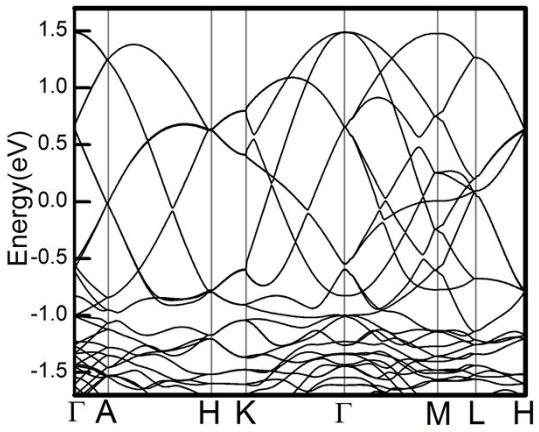

Figure s1, Band structure of $LaCuO_3$ calculated by the PBE+SOC method. The Fermi level is set to zero.

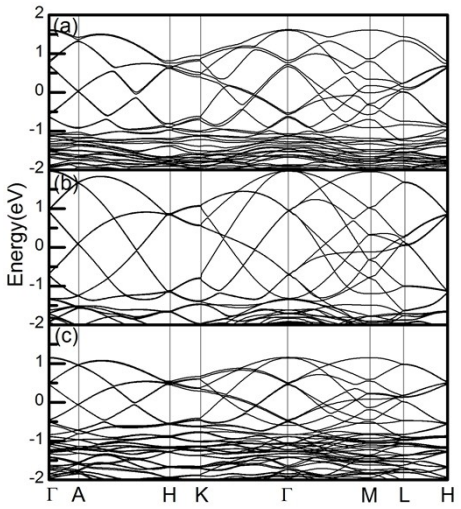

Figure s2, The band structures of $LaCuO_3$ calculated using (a) experimental lattice parameter, (b) under -5% strain, and (c) under +5% strain.

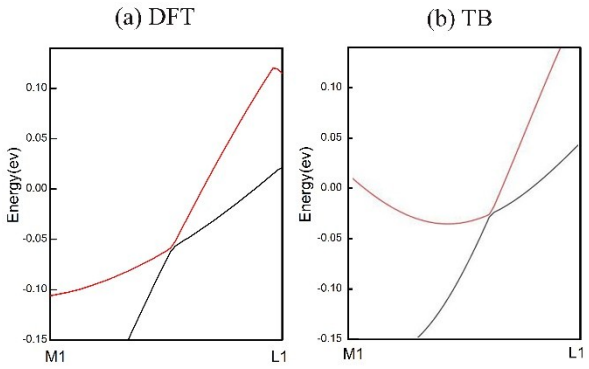

Figure s3, The band structures of $LaCuO_3$ along M1-L1 line calculated by (a) HSE06 and (b) TB model.

The tight-binding Hamiltonian for $LaCuO_3$ in a localized basis set is as follows,

$$H = -\sum_{ij}\left(t_{ij}c_i^+ c_j + h.c.\right) + \sum_i \epsilon_i c_i^+ c_i$$

where ϵ_i is the on-site energy, t_{ij} is the hopping integral and c_i^+/c_i is the fermion creation/annihilation operator at site i. By Fourier transform to momentum space, we can obtain the matrix elements of the Hamiltonian in the Bloch basis set,

$$H_{ij}(\vec{k}) = -\sum_{\vec{R}} e^{i\vec{k}\vec{R}}\langle \vec{r},i \,|\, \vec{r}-\vec{R},j\rangle$$

here $\vec{k}$ is the wave vector, $\vec{r}$ is the position of *i*th primitive cell, $\vec{R}$ is the relative position of *j*th atom to the primitive cell . As the dominant contributions to valence and conduction band at the Dirac cone 7 (distorted Dirac cone) is from the hybridization of dyz and $d_{x^2-y^2}$ orbitals of Cu atoms, and the 6 Cu atoms in the unit cell contributes equally to cone 7. We simplify the TB model by using one Cu atom (set atomic position as (0, 0, 0)) and two orbitals (dyz and $d_{x^2-y^2}$). Six nearest Cu atoms with relative atomic coordinates ($1.6, 2.77, 8.74$), (3.20, 5.54, 4.37), ($3.20, 0, 4.37$), ($7.99, 2.77, 4.37$), (6.39, 0, 8.74), and (6.39, 5.54, 8.74), respectively.

Figure s4 shows that the van der waals dispersion has neglectable effect on the band structure of $LaCuO_3$.

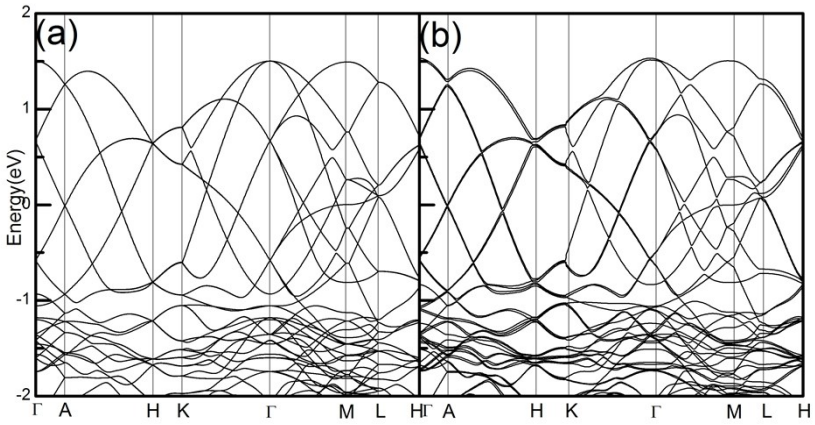

Figure s4, The band structures of $LaCuO_3$ calculated using PBE method (a) with van der waals force and (b) without van der waals force.

Figure s5 demonstrates that the Dirac cones in the Γ-A-H-K-Γ plane are linearly dispersed in three directions for $LaCuO_3$. In Γ-A-H-K-Γ plane, the value of kx equals to the value of ky.

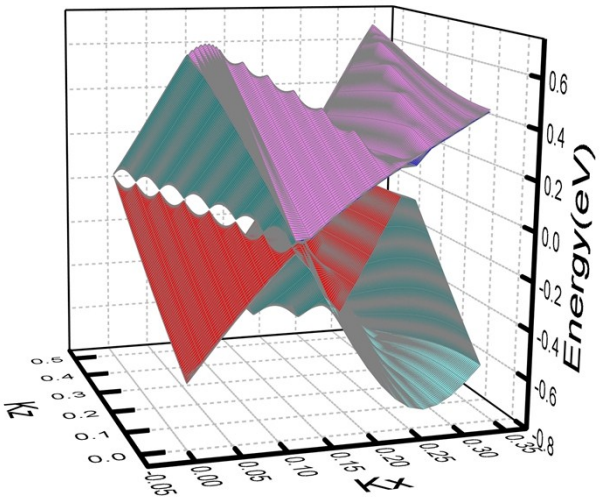

Figure s5, 3D band structure plot of LaCuO3 in the Γ-A-H-K-Γ plane in the first BZ.