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.
The band structures of LaCuO$_3$ calculated using (a) experimental lattice parameter, (b) under -5% strain, and (c) under +5% strain.

The tight-binding Hamiltonian for LaCuO$_3$ in a localized basis set is as follows,

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

where \( \epsilon_i \) 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,

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

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 \( d_{yz} \) 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 (\( d_{yz} \) 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 $\Gamma$-A-H-K-$\Gamma$ plane are linearly dispersed in three directions for LaCuO$_3$. In $\Gamma$-A-H-K-$\Gamma$ plane, the value of $k_x$ equals to the value of $k_y$.

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