Ab initio derivation of effective low-energy model of $Ca_5Ir_3O_{12}$

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In this report, we report a first-principles derivation of an effective low-energy model for $Ca_5Ir_3O_{12}$. In order to perform the effective-model derivation of materials with strong spin-orbit interaction (SOI) such as iridium system, we extended the first principle effective-model derivation software RESPACK [1] to the spinor type.

The density-functional band-structure calculations for $Ca_5Ir_3O_{12}$ are performed using xTAPP [2] with the experimental lattice parameters [3]: $a = 9.3490$ Å and $c = 3.1713$ Å. We use the norm-conserving pseudopotential and the generalized gradient approximation (GGA) of the exchange correlation potential. We use 8×8×8 k-points for sampling in the first Brillouin zone. The energy cutoff is set to be 144 Ry for the wave functions, and 576 Ry for the charge density. The interaction parameters are calculated using the constrained random-phase approximation method, in which we employ the scheme for the band disentanglement. The energy cutoff for the dielectric function is set to be 20 Ry. The total number of bands used in the calculation of the polarization is 300, which includes the unoccupied states up to $\sim$ 26 eV with respect to the Fermi level. To study the effects of SOI, we performed the usual GGA calculation and compared it with the result including the SOI. Below, we refer to the former as GGA and to the latter as SO-GGA.

From the fat band analysis, it was found that the band structure near the Fermi energy is d_{xy} and d_{yz} orbitals. Here, the notation of the orbital follows a local coordinate system fixed to the IrO_6 octahedron. Based on this observation, we perform parameter derivation of the d_{xy}/d_{yz} model. Figure 1 is a comparison of the Wannier-interpolation band (green-dashed curves) and the original band (red-solid curves). We see that the original band has been completely reproduced. Note that the initial guess setting is very important for obtaining such reproducibility. We set the d_{xy} and d_{yz} orbitals as initial guesses, where the initial guess orbitals are represented in the local coordinate system fixed to IrO_6 octahedrons, and additionally rotated the spin quantization axis. This treatment is very important to satisfy the symmetry of the calculated Wannier orbitals, that is, all 12 Wannier orbitals have the same spread.

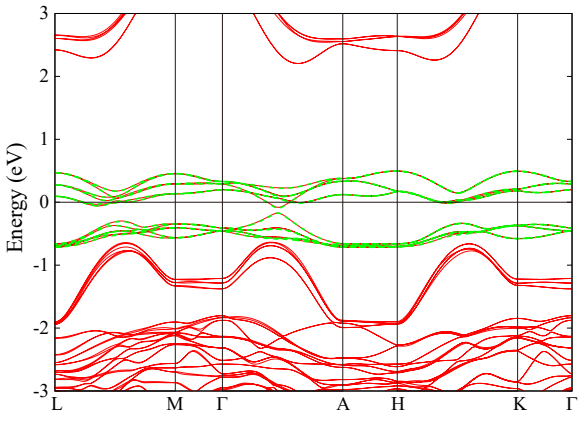

Figure 1: (a) *Ab initio* density functional band structure considering the spin-orbit interaction in $Ca_5Ir_3O_{12}$.

We next show in Fig. 2 the resulting maximally localized Wannier functions for d_{xy}/d_{yz} model. The panels (a) and (b) indicate the d_{xy} and d_{yz} Wannier functions, respectively. Note that in this plot, three independent Wannier functions are shown in one panel.

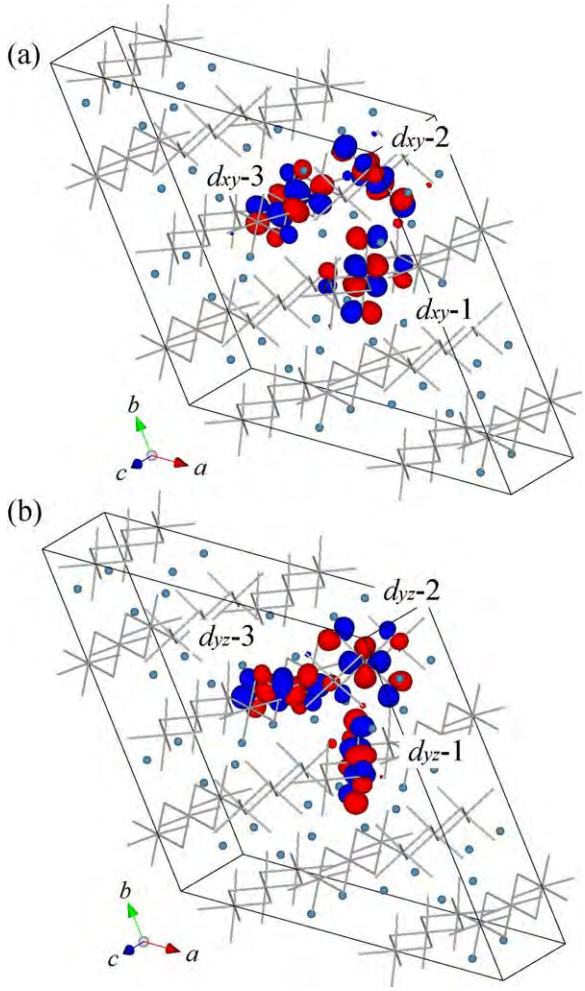

Figure 2: Maximally localized Wannier functions of $Ca_5Ir_3O_{12}$: (a) d_{xy} and (b) d_{yz} Wannier functions.

Our derived model parameters for $Ca_5Ir_3O_{12}$ are summarized in the Table 1. The spin-orbit coupling is estimated as 0.213 eV. The nearest neighbor parameter t_{NN} is 0.167 eV, the onsite interaction U based on constraind RPA is 2.43 eV, and the nearest-neighbor interaction V is estimated as 0.99 eV. Then, the correlation degree of freedom $(U-V)/t$ is 8.62.

Table 1: Main parameters of d_{xy}/d_{yz} model of $Ca_5Ir_3O_{12}$, where we show 3 nearest-neighbor (NN) transfers, onsite transfers, and largest interchain electron transfer. $t^{NN}_{xy\uparrow,yz\uparrow}$ and $t^{NN}_{yz\uparrow,xy\uparrow}$ are nearest neighbor trasnfers. Also, $t^{onsite}_{xy\uparrow,yz\downarrow}$ is the spin-orbital couplings in the same site. The interaction parameters with the bare (unscreened) and constrained RPA (cRPA) are listed. $V_{\rm NN}$ is the orbital-averaged value of the nearest-neighbor interactions. Also, $V_{\rm IC}$ is the orbital-averaged value of the interchaicn interaction. The unit of the parameters is eV.

	SO-GGA		GGA	
$t^{NN}_{xy\uparrow,yz\uparrow}$	0.167		0.167	
$t^{NN}_{yz\uparrow,xy\uparrow}$	0.210		0.208	
$t^{largest}_{interchain}$	0.032		0.039	
$t^{onsite}_{xy\uparrow,yz\downarrow}$	0.213		-	
	bare	cRPA	bare	cRPA
U	9.87	2.43	10.03	2.23
U'	9.19	1.95	9.28	1.68
V_{NN}	4.43	0.99	4.39	0.77
$V_{interchain}$	2.86	0.52	2.86	0.44
J	0.27	0.21	0.29	0.23

As another achievement, we calculated the Raman frequency [4] and the phonon dispersion curves [5].

References

[1] https://sites.google.com/view/kazuma7k6r

[2] http://xtapp.cp.is.s.u-tokyo.ac.jp

[3] M. Wakeshima, N. Taira, Y. Hinatsu, and Y. Ishii, Solid State Commun. **125**, 311 (2003).

[4] T. Hasegawa, W. Yoshida, K. Nakamura, N. Ogita, and K. Matsuhira:: J. Phys. Soc. Jpn **89** (2020) 054602/1-11.

[5] H. Hanate, T. Hasegawa, S. Tsutsui, K. Nakamura, Y. Yoshimoto, N. Kishigami, S. Haneta, and K. Matsuhira1: J. Phys. Soc. Jpn **89** (2020) 053601/1-5.