

supplemental material for

New two-dimensional flat band materials: $B_3C_{11}O_6$ and $B_3C_{15}O_6$

Jialuo Dong,¹ Pan Zhou,^{1,*} Yuzhong Hu,¹ and Lizhong Sun^{1,†}

¹Hunan Provincial Key laboratory of Thin Film Materials and Devices,
School of Material Sciences and Engineering, Xiangtan University, Xiangtan 411105, China

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I. STRUCTURAL EVOLUTION FROM KAGOME TO KAGOME-1 AND KAGOME-2

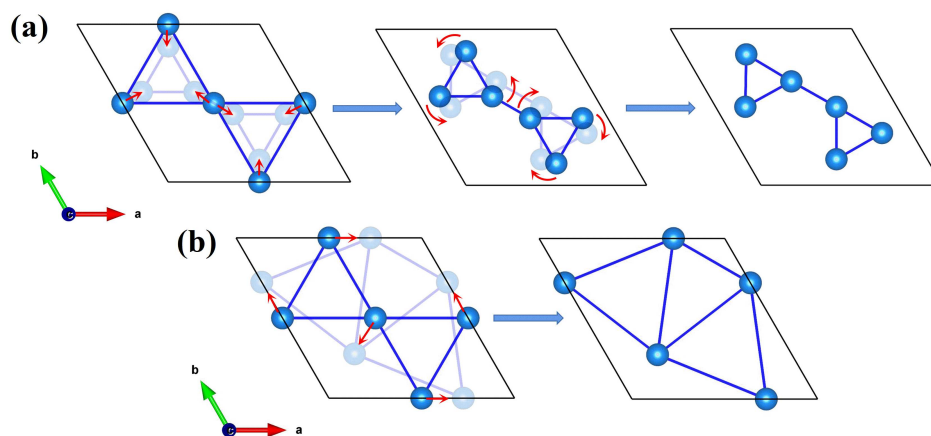


Figure S1: Structural evolution from kagome to (a) kagome-1 and (b) kagome-2.

II. KAGOME-1 AND DISTORTED KAGOME-1 AND CORRESPONDING ENERGY BAND STRUCTURE

Figures S2(a) and S2(b), respectively, are the crystal structures of kagome-1 and distorted kagome-1. Their energy band structures with the parameters of $t_1 = -1.0$ and $t_2 = -1.0$ are shown in Fig. S2(c) and S2(d). It is revealed that their energy bands share the similar characteristic of dispersion.

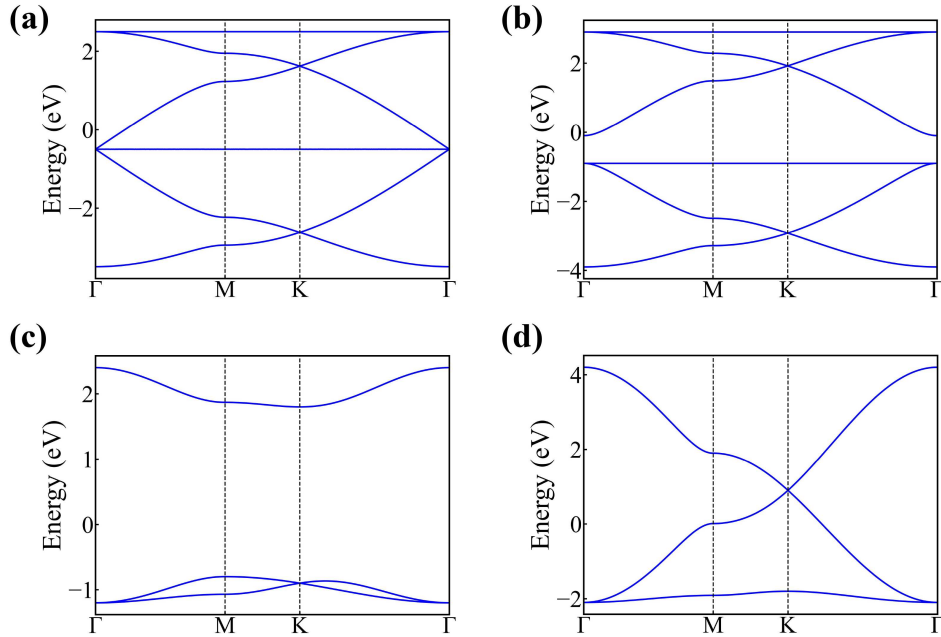


Figure S2: (a) and (b) are two structures of kagome-1 respectively, where $t_1 = -1.0$ and $t_2 = -1.0$. (c) and (d) correspond to their energy bands respectively.

We can obtain three typical energy band dispersions in the kagome-1 lattice by adjusting the parameters t_1 and t_2 . The band structure is shown in Fig. 1(e) of the main text when $t_2 < \frac{3t_1}{2}$. Here, we present the band structure at $t_2 = \frac{3t_1}{2}$ and $t_2 > \frac{3t_1}{2}$ in Fig. S3(a) and S3(b), respectively. We provide the band structure for kagome-2 lattice that only takes into account t_1 and t_2 . The band structure is presented as two crossed bands and one isolated band with apparent dispersion when $t_1 > t_2$ [see Fig. S3(c)]. However, since the focus of our research is on the flat band's physical characteristics, adding the third nearest neighbor results in a flat band with virtually no bandwidth [see Fig. 1(f) of the main text]. Additionally, the band structure of the kagome-2 lattice is nearly identical to that of the Kagome lattice when we make $t_2 \gg t_1$, as shown in Fig. S3(d).

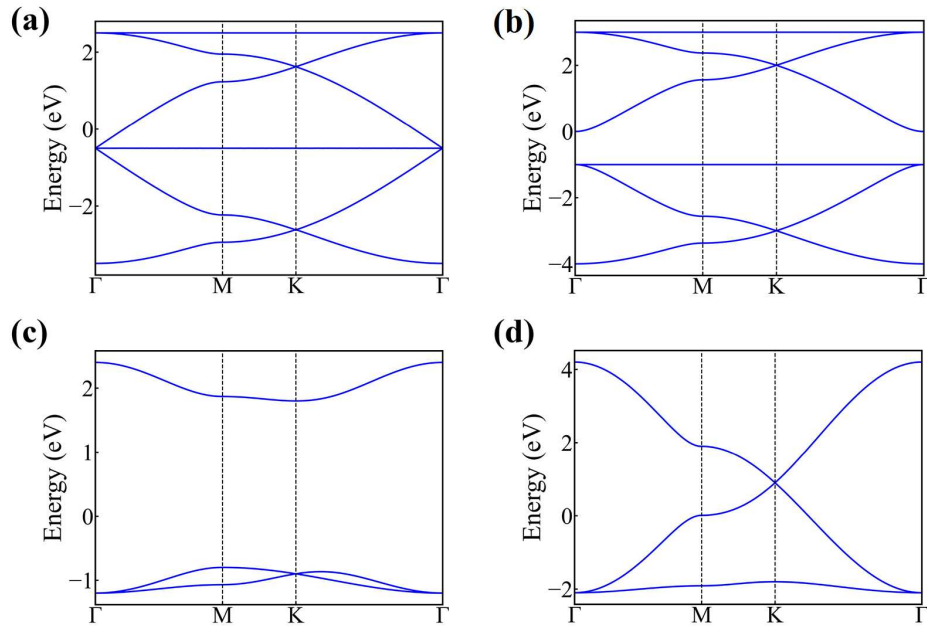


Figure S3: The energy band structure of kagome-1 lattice with (a) $t_1 = -1.0$ and $t_2 = -1.5$, and (b) $t_1 = -1.0$ and $t_2 = -2.0$. The energy band structure of kagome-2 lattice with (c) $t_1 = 1.0$ and $t_2 = 0.1$, and (d) $t_1 = -0.1$ and $t_2 = -1.0$.

* Electronic address: zhoupan71234@xtu.edu.cn

† Electronic address: lzsun@xtu.edu.cn