

Supporting Information

K₁₁Cd₂Sb₅ Built of Unprecedented Planar CdSb₃

Triangle

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1. Experimental Section

1.1 Synthesis

All the chemicals were obtained from commercial sources and was handled in N₂ atmosphere using an N₂-filled glovebox. K was purified by liquating, Cd granules (99.99%, ChemPur) and Bi granules (99.99%, ChemPur) were used as received.

K₁₁Cd₂Sb₅ are synthesized by reactions of the stoichiometric proportions of the elements in welded niobium containers that were sealed in an evacuated fused silica jacket (20 mm i.d.) under high vacuum (ca. 10⁻³ Pa). The assembly were heated at 700 °C for 48 hours and then cooled to room temperature with the cooling rate of 5 °C h⁻¹.

1.2 The data collection

The intensity data were collected on a Rigaku Mercury CCD diffractometer with graphite-monochromated MoK α radiation ($\lambda = 0.71073 \text{ \AA}$) at room temperature. All absorption corrections were performed using multiscan. The structure was solved by direct methods and refined by full-matrix least-squares on F² with the SHELXTL-97¹ program package.

1. Sheldrick, G. M. SHELXTL, version 6.21; Bruker-Nonium AXS: Madison, WI, 2001.

1.3 X-ray Powder Diffraction

The samples were assessed for phase purity using powder X-ray diffraction. PXRD pattern were collected on a Rigaku DMAX 2500 powder diffractometer with ultra 18 Kw Cu K α radiation. The sample of K₁₁Cd₂Sb₅ is protected by the Magic Tape when they were tested. The dates are treated by jade 6.0.

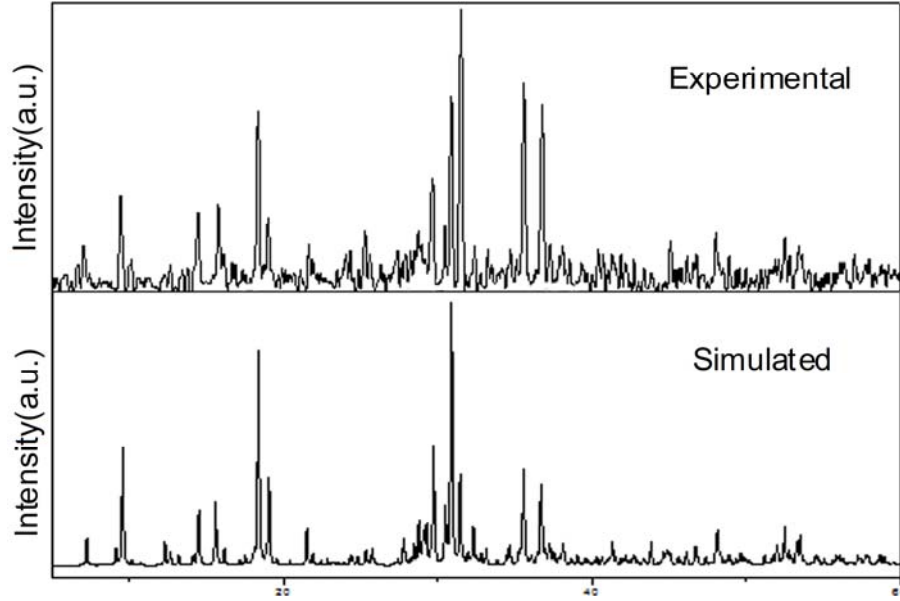


Fig. S1. Experimental and simulated X-ray powder diffraction patterns of $K_{11}Cd_2Sb_5$.

1.5 Computational descriptions

Band structures and density of states (DOS) are calculated by the projector augmented wave (PAW) method¹ implemented in the Vienna ab initio simulation package (VASP)². The exchange-correlation functional is the Perdew-Burke-Ernzerhof (PBE)³. The PAW potentials are used with the following valence-electron configurations: $3s^23p^64s^1$ for K, $4d^{10}5s^2$ for Cd, and $5s^25p^3$ for Sb atom. The plane-wave cutoff energy of 300 eV and the threshold of 10^{-5} eV are used for the self-consistent-field convergence of the total electronic energy. Monkhorst-Pack mesh of $3 \times 3 \times 3$ in electronic structure calculation is used.

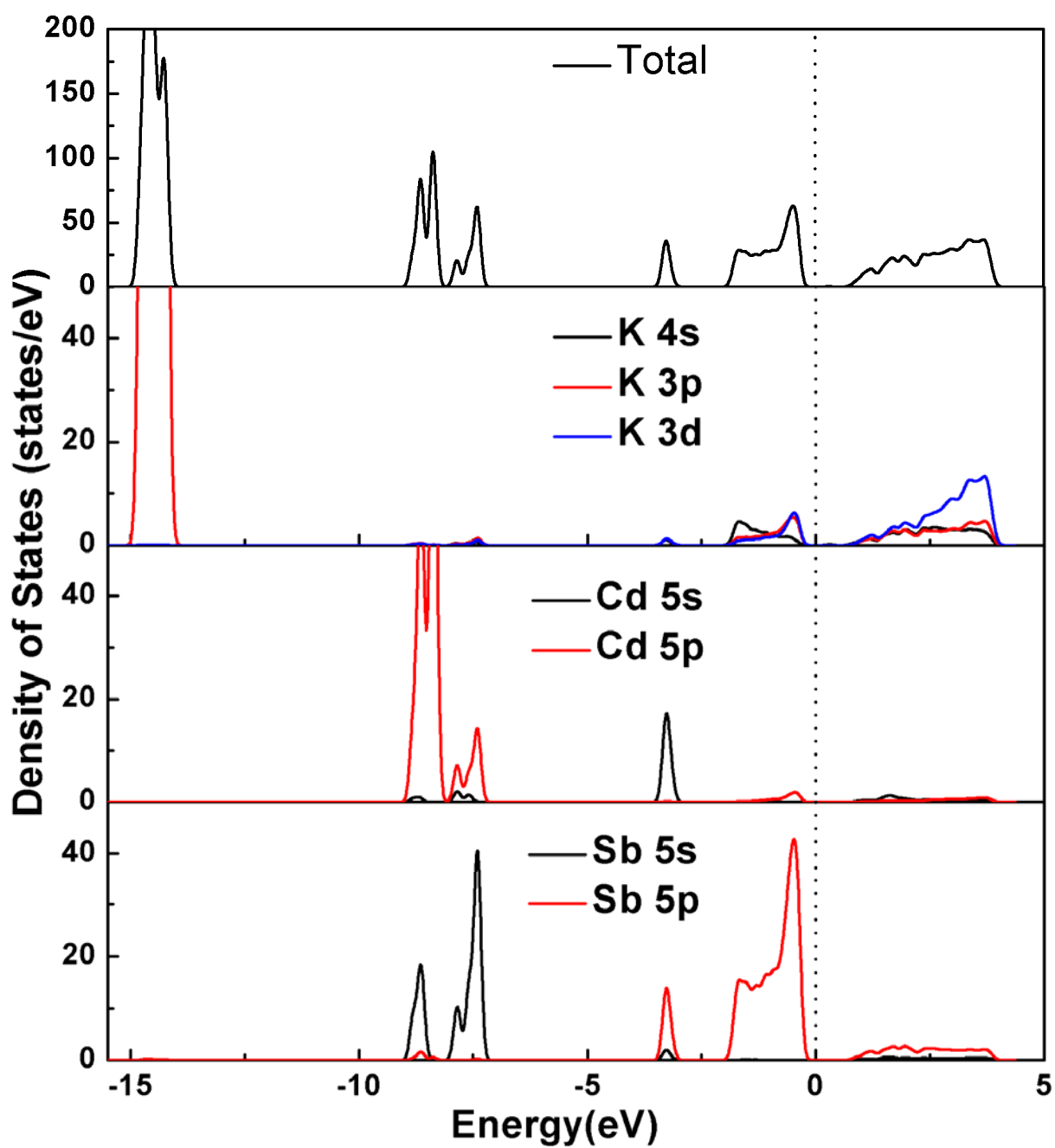


Fig. S2 Total and partial density of states of 1.

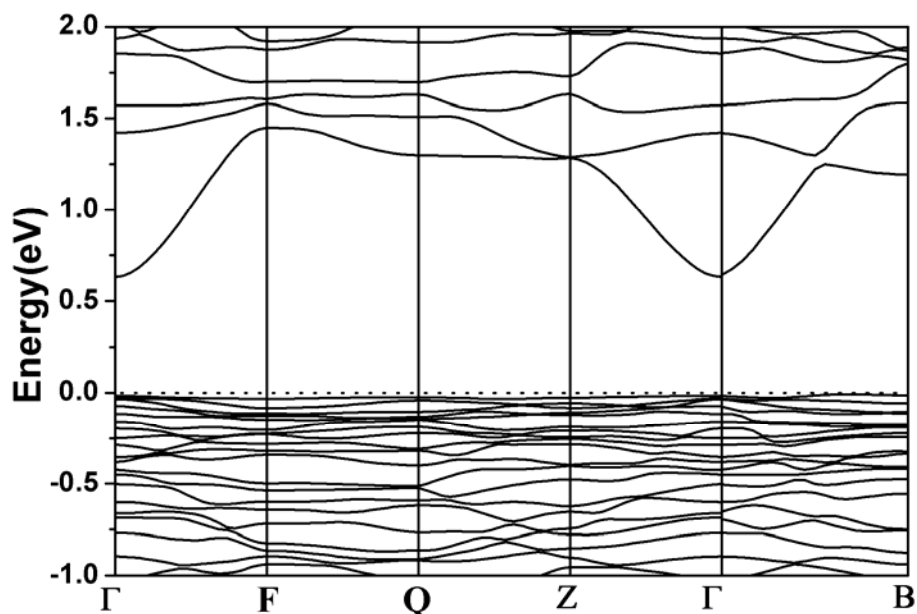


Fig. S3 Calculated band structure of **1**, the Fermi level is set to 0 eV.

1. Blöchl, P. E. *Physical Review B* 1994, **50**, 17953.
2. Kresse, G.; Furthmüller, J. *Physical Review B* 1996, **54**, 11169.
3. Perdew, J. P.; Burke, K.; Ernzerhof, M. *Physical Review Letters* 1996, **77**, 3865.

2. Tables

Table S1 Details of the powder X-ray diffraction measurement and Rietveld refinement of the crystal structure of $K_{11}Cd_2Sb_5$.

Formula	$K_{11}Cd_2Sb_5$
Formula mass (amu)	1263.65
Crystal system	Triclinic
Space group	P-1 (NO.2)
Cell parameters	$a=9.9138(13) \text{ \AA}$, $\alpha=103.570(4)^\circ$ $b=12.0122(17) \text{ \AA}$, $\beta=97.304(3)^\circ$ $c=12.8485(17) \text{ \AA}$, $\gamma=107.615(4)^\circ$
Volume	$1384.8(3) \text{ \AA}^3$
Formula units per cell	$Z=2$
Calculated density	3.030 Mg/m^3
Temperature/K	293(2)
Absorption coefficient	7.945 mm^{-1}
Theta range for data collection	2.34 to 24.50 deg
Limiting indices	$-11 \leq h \leq 11$, $-13 \leq k \leq 13$, $-14 \leq l \leq 14$
Goodness-of-fit on F^2	1.066
Completeness to theta = 25.00	95.2%
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0430$, $wR_2 = 0.1134$
R indices (all data)	$R_1 = 0.0529$, $wR_2 = 0.1330$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{K}_{11}\text{Cd}_2\text{Sb}_5$.

atom	x	y	z	U _{eq} (\AA)
Sb(1)	9995(1)	2351(1)	4444(1)	17(1)
Sb(2)	13393(1)	5438(1)	3079(1)	19(1)
Cd(2)	10537(1)	421(1)	2812(1)	20(1)
Cd(1)	10538(1)	3753(1)	2848(1)	19(1)
Sb(4)	13371(1)	277(1)	3005(1)	18(1)
Sb(5)	8078(1)	-1474(1)	1346(1)	18(1)
Sb(3)	8101(1)	3686(1)	1352(1)	18(1)
K(1)	11420(4)	4254(3)	356(3)	28(1)
K(2)	6927(3)	1054(3)	2228(3)	26(1)
K(3)	13649(3)	8333(3)	4694(3)	29(1)
K(4)	13671(3)	3264(3)	4403(3)	25(1)
K(5)	7940(4)	4414(3)	4281(3)	33(1)
K(6)	9498(4)	2944(3)	7315(3)	38(1)
K(7)	7947(4)	-795(3)	4289(3)	34(1)
K(8)	11242(4)	-944(3)	156(3)	31(1)
K(9)	14138(4)	-2273(3)	1360(3)	31(1)
K(10)	6067(4)	-2481(3)	-1409(3)	38(1)
K(11)	16516(5)	5885(4)	2099(5)	58(1)

^a U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Select bond distances (\AA) and angles ($^\circ$) for $\text{K}_{11}\text{Cd}_2\text{Sb}_5$.

Sb(1)-Cd(1)	2.9462(15)
Sb(1)-Cd(2)	2.9698(13)
Sb(2)-Cd(1)	2.8691(14)
Cd(2)-Sb(4)	2.8502(14)
Cd(2)-Sb(5)	2.8516(13)
Cd(1)-Sb(3)	2.8581(13)
Cd(1)-Sb(1)-Cd(2)	84.84(4)
Sb(4)-Cd(2)-Sb(5)	122.02(4)
Sb(4)-Cd(2)-Sb(1)	119.54(4)
Sb(5)-Cd(2)-Sb(1)	117.49(4)
Sb(3)-Cd(1)-Sb(2)	121.82(5)
Sb(3)-Cd(1)-Sb(1)	118.11(4)
Sb(2)-Cd(1)-Sb(1)	119.21(4)

3. Figures of crystal and coordination structures

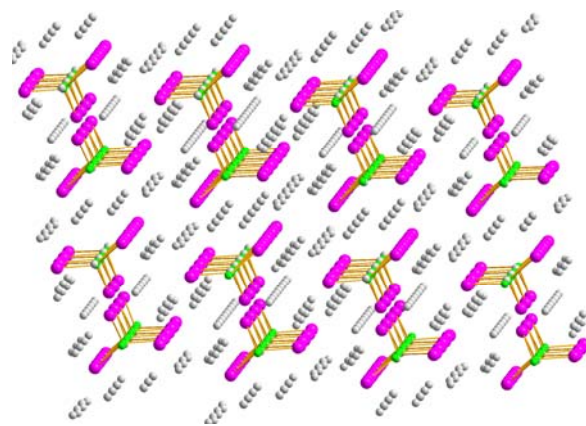


Fig. S4. Crystal structures of 1.

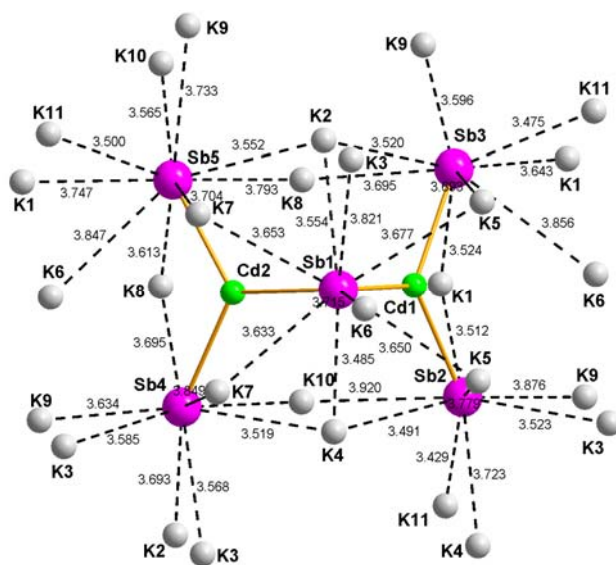


Fig. S5 Interactions between K and Sb.

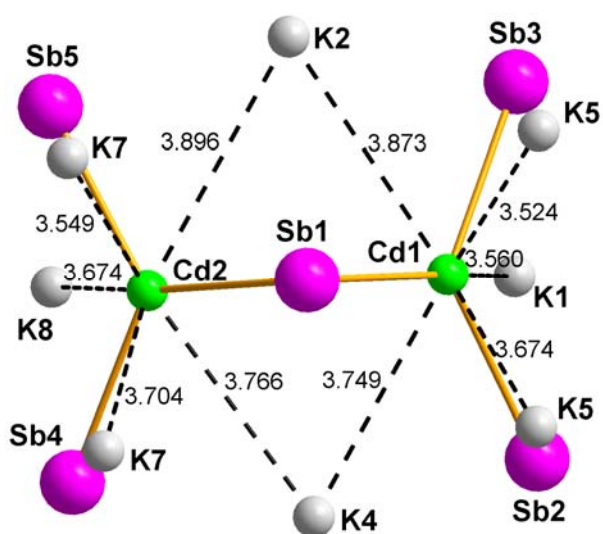


Fig. S6 Interactions between Cd and K.

Reference

- 22 Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, Jr., T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, revision D.02. Gaussian, Inc., Wallingford CT, 2004.