

Supporting Information

Intermetallic Compounds with 1D Infinite Tunnels. Syntheses and Structures of $A\text{Au}_4\text{In}_2$ ($A = \text{K}, \text{Rb}$)

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Table S1 Single Crystal and Structural Refinements Data for $\text{K}_x\text{Rb}_{1-x}\text{Au}_4\text{In}_2$ ($x = 1, 0.87, 0.65, 0$).

Compound	(I) KAu_4In_2	(II) $\text{K}_{0.87(7)}\text{Rb}_{0.13}\text{Au}_4\text{In}_2$	(III) $\text{K}_{0.65(9)}\text{Rb}_{0.35}\text{Au}_4\text{In}_2$	(IV) RbAu_4In_2
Formula weight	1056.61	1062.63	1072.84	1102.98
Space group, Z	$I4/mcm$ (No. 140), 4			
Temperature	293(2) K			
Wavelength	0.71073 Å			
a (Å) ^a	8.668(1)	8.703(1)	8.785(1)	8.835(1)
c (Å)	8.368(2)	8.337(2)	8.326(2)	8.274(3)
V (Å ³)	628.7(2)	631.5(2)	642.6(2)	645.8(2)
d_{cal} (g/cm ³)	11.163	11.177	11.089	11.344
Theta range for data collection	3.32 to 29.05°	3.31 to 28.71	3.28 to 28.65°	3.26 to 29.32°
abs. coeff (mm ⁻¹)	100.725	101.187	100.952	104.899
Data / restraints / parameters	248 / 0 / 14	239 / 0 / 15	245 / 0 / 15	259 / 0 / 14
Goodness-of-fit on F^2	1.028	1.350	1.094	1.247
$R1/wR2$ [$I > 2\sigma(I)$]	0.0411/ 0.1060	0.0396/ 0.0691	0.0479/ 0.1128	0.0540/ 0.1299
$R1/wR2$ [all data]	0.0744/ 0.1116	0.0731/ 0.0732	0.0735/ 0.1226	0.0832/ 0.1363
peak/ hole (e/ Å ⁻³)*	3.576 and -2.959	3.342 and -1.597	4.023 and -2.395	6.000 and -3.089

* All peaks are close to Au at distance of less than 1 Å.

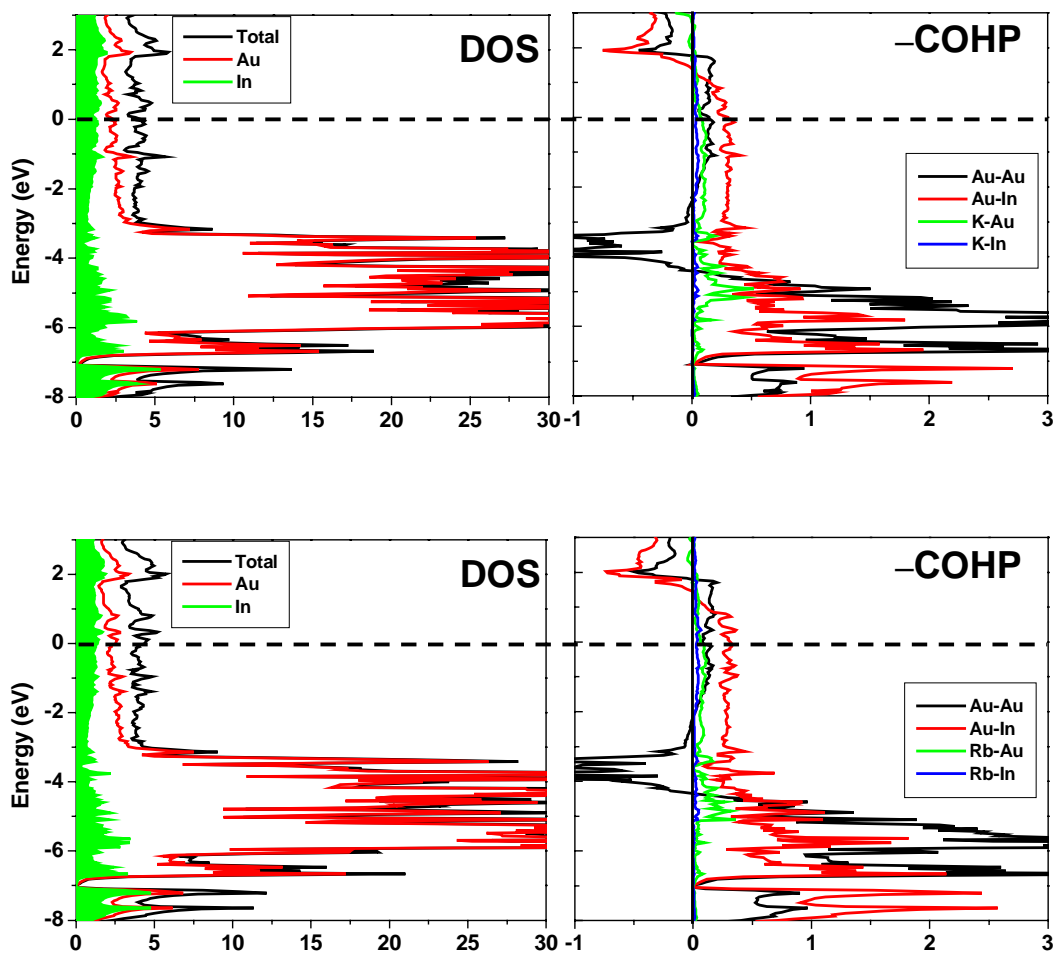


Figure S1 TB-LMTO-ASA electronic structure calculation results for KAu_4In_2 (top) and RbAu_4In_2 (bottom). Left: Total DOS (black) and separate partial DOS curves for indium (green) and gold (red). Right: $-\text{COHP}$ data for the interactions: Au-Au; Au-In; A-Au; and A-In (A = K, Rb). The dotted lines denote the Fermi levels.