Supporting Information

Clathrate $Ba_8Au_{16}P_{30}$: The "Gold Standard" for Lattice Thermal Conductivity

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Table SI 1. Atomic coordinates and isotropic displacement parameters for $Ba_8Au_{16}P_{30}$.

Atom	Site	x/a	y/b	z/c	U_{so}
Ba1	4*b*	0	0.5	0	0.0139(8)
Ba2	4*c*	0	0.0062(3)	0.25	0.0125(8)
Ba3	8*d*	0.3757(2)	0.9915(3)	0.18733(9)	0.0287(7)
Ba4	8*d*	0.1246(2)	0.0085(3)	0.06050(9)	0.0224(7)
Ba5	8*d*	0.2486(2)	0.2540(3)	0.3763(1)	0.0256(6)
Au1	8*d*	0.1858(1)	0.1889(2)	0.24960(6)	0.0180(4)
Au2	8*d*	0.0020(1)	0.3196(2)	0.09348(5)	0.0180(4)
Au3	8*d*	0.3799(1)	0.0045(2)	0.31054(5)	0.0224(4)
Au4	8*d*	0.5522(1)	0.3159(2)	0.03118(6)	0.0185(4)
Au5	8*d*	0.9014(1)	0.0037(2)	0.14210(5)	0.0180(4)
Au6	8*d*	0.7164(1)	0.0100(2)	0.04688(5)	0.0163(4)
Au7	8*d*	0.6523(1)	0.3810(2)	0.32760(6)	0.0228(5)
Au8	8*d*	0.1612(1)	0.6155(2)	0.07944(6)	0.0182(5)
P1	8*d*	0.0050(7)	0.192(1)	0.1603(3)	0.0049(5)
P2	8*d*	0.4863(7)	0.309(0)	0.3402(3)	0.0049(5)
P3	8*d*	0.6835(7)	0.192(1)	0.9980(3)	0.0049(5)
P4	8*d*	0.1881(7)	0.679(1)	1.0002(3)	0.0049(5)
P5	8*d*	0.4990(8)	0.179(1)	0.0951(3)	0.0049(5)
P6	8*d*	0.2481(9)	0.260(1)	0.1243(4)	0.0049(5)
P7	8*d*	0.5623(6)	0.69631)	0.0304(4)	0.0049(5)
P8	8*d*	0.5969(6)	0.004(1)	0.1063(3)	0.0049(5)
P9	8*d*	0.2132(6)	0.011(1)	0.2961(3)	0.0049(5)
P10	8*d*	0.1822(6)	0.817(1)	0.2570(3)	0.0049(5)
P11	8*d*	0.1237(6)	0.018(1)	0.4414(3)	0.0049(5)
P12	8*d*	0.1523(7)	0.125(0)	0.1694(3)	0.0049(5)
P13	8*d*	0.5537(6)	0.808(1)	0.2209(3)	0.0049(5)
P14	8*d*	0.1528(7)	0.3690(9)	0.0769(4)	0.0049(5)
P15	8*d*	0.0661(7)	0.7074(9)	0.2830(3)	0.0049(5)

Table SI 2. Selected interatomic distances in $Ba_8Au_{16}P_{30}$.

Atoms		*d*, Å	Atoms		*d*, Å
Ba1	Au2	3.302(2)	Au1	P9	2.34(1)
Ba1	Au4	3.511(2)	Au1	P10	2.36(1)
Ba1	Au6	3.448(1)	Au1	P13	2.46(1)
Ba1	Au8	3.511(2)	Au1	P12	2.47(1)
Ba1	P3	3.36(1)	Au2	P1	2.35(1)
Ba1	P4	3.33(1)	Au2	P7	2.43(1)
Ba1	P5	3.34(1)	Au2	P8	2.45(1)
Ba1	P7	3.42(1)	Au2	P14	2.32(1)
Ba1	P8	3.391(8)	Au3	P8	2.44(1)
Ba1	P14	3.44(1)	Au3	P9	2.48(1)
Ba1	P14	3.44(1)	Au3	P13	2.46(1)
Ba2	Au1	3.325(3)	Au3	P15	2.39(1)
Ba2	Au5	3.444(1)	Au4	P3	2.51(1)
Ba2	Au7	3.427(2)	Au4	P5	2.47(1)
Ba2	P1	3.25(1)	Au4	P7	2.45(1)
Ba2	P2	3.32(1)	Au4	P11	2.50(1)
Ba2	P9	3.393(9)	Au5	P1	2.54(1)
Ba2	P10	3.33(1)	Au5	P2	2.42(1)
Ba2	P13	3.36(1)	Au5	P9	2.45(1)
Ba2	P12	3.46(1)	Au5	P11	2.45(1)
Ba2	P15	3.43(1)	Au6	P3	2.42(1)
Ba3	Au1	3.755(4)	Au6	P4	2.44(1)
Ba3	Au2	3.721(3)	Au6	P8	2.45(1)
Ba3	Au3	3.573(3)	Au6	P11	2.36(1)
Ba3	Au3	3.580(3)	Au7	P2	2.58(1)
Ba3	Au7	3.496(3)	Au7	P6	2.38(1)
Ba3	Au8	3.428(3)	Au7	P10	2.58(1)
Ba3	P13	3.38(1)	Au7	P12	2.55(1)
Ba3	P13	3.44(10	Au8	P4	2.43(1)
Ba3	P14	3.48(10	Au8	P5	2.48(1)
Ba4	Au2	3.839(3)	Au8	P6	2.39(1)
Ba4	Au4	3.401(3)	Au8	P14	2.58(1)
Ba4	Au4	3.389(3)	P1	P13	2.30(1)
Ba4	Au7	3.530(3)	P1	P12	2.28(1)
Ba4	Au8	3.374(3)	P2	P5	2.33(1)
Ba4	P7	3.48(1)	P2	P15	2.12(1)
Ba4	P11	3.463(9)	P3	P4	2.31(1)
Ba4	P12	3.40(1)	P3	P14	2.30(1)
Ba5	Au1	3.844(3)	P4	P7	2.42(1)

Ba5	Au2	3.832(4)	P5	P8	2.35(1)
Ba5	Au3	3.760(3)	P6	P12	2.38(1)
Ba5	Au3	3.746(3)	P6	P14	2.27(1)
Ba5	Au5	3.458(4)	P7	P11	2.22(1)
Ba5	Au5	3.482(4)	P9	P10	2.36(1)
Ba5	Au6	3.427(3)	P10	P15	2.18(1)
Ba5	Au6	3.516(3)	P13	P13	2.30(1)
Ba5	P8	3.49(1)	P15	P15	2.72(2)
Ba5	P8	3.47(1)			
Ba5	P9	3.49(1)			

Table SI 3. Au–P bond distance, gold coordination number (CN) and shape of AuP_n fragments in the selected inorganic compounds.

Compound	d(Au–P), Å	Au CN	AuP_n fragment	Reference
$Au(PF_3)_2^+$	2.25	2	linear	S1
Au_2P_3	2.33-2.34	2	linear	23
MAu_2P_2 (M = Hg, Tl, Pb)	2.33-2.34	2	linear	S2
K_5AuP_2	2.37	2	linear	S3
K_2AuP	2.40	2	linear	S4
$BaAu_2P_4$	2.36	2	linear	16
$Au_7P_{10}I$	2.32-2.34	2, 3	linear, trigonal planar	S5
CaAuP	2.45	3	trigonal planar	S6
EuAuP	2.49	3	trigonal planar	S7
BaAuP	2.54	3	trigonal planar	S8
La_2AuP_2O	2.42-2.48	3	trigonal planar	31b, S9
Au_3SnP_7	2.41-2.55	3	trigonal pyramid	S10
R_2AuP_3 (R = Ce, Pr, Nd)	2.46-2.53	3	tetrahedral	S11
$Au_{1-x}Sn_{1+x}P_{14}$	2.46-2.53	4	tetrahedral	S12
$Ba_8Au_{16}P_{30}$	2.34-2.58	4	tetrahedral	*current work*

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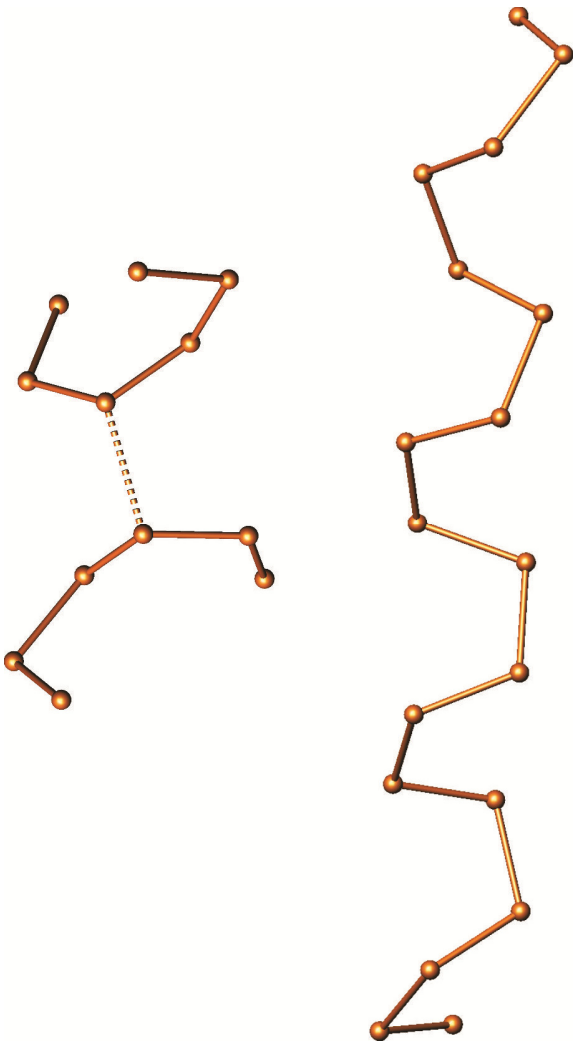

Figure SI 1. P_{12} (left) and P_{18} (right) polyphosphide fragments in the crystal structure of $Ba_8Au_{16}P_{30}$.

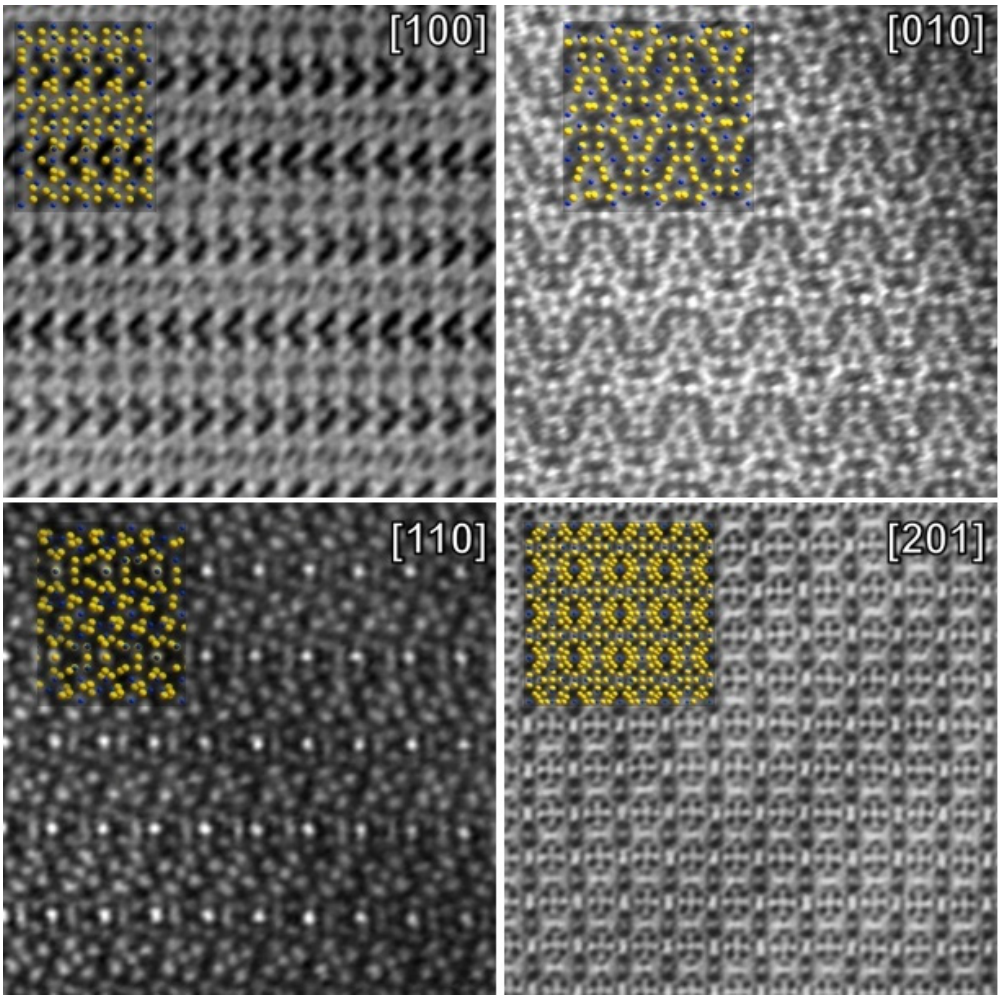

Figure SI 2. High resolution HAADF-STEM images along main zone axis and corresponding overlay structural model of $Ba_8Au_{16}P_{30}$. Only Au (yellow) and Ba(blue) atoms shown for clarity.

Table SI 4. Chemical shifts and relative intensity of the ^{31}P NMR signals for $Ba_8Cu_{16}P_{30}$.

Type of P atoms	Structural ratio	δ, ppm
1*b*-P: 3Cu+P	6	132 and 388
2*b*-P: 2Cu+2P	22	710 and 364
3*b*-P: 1Cu+3P	2	51

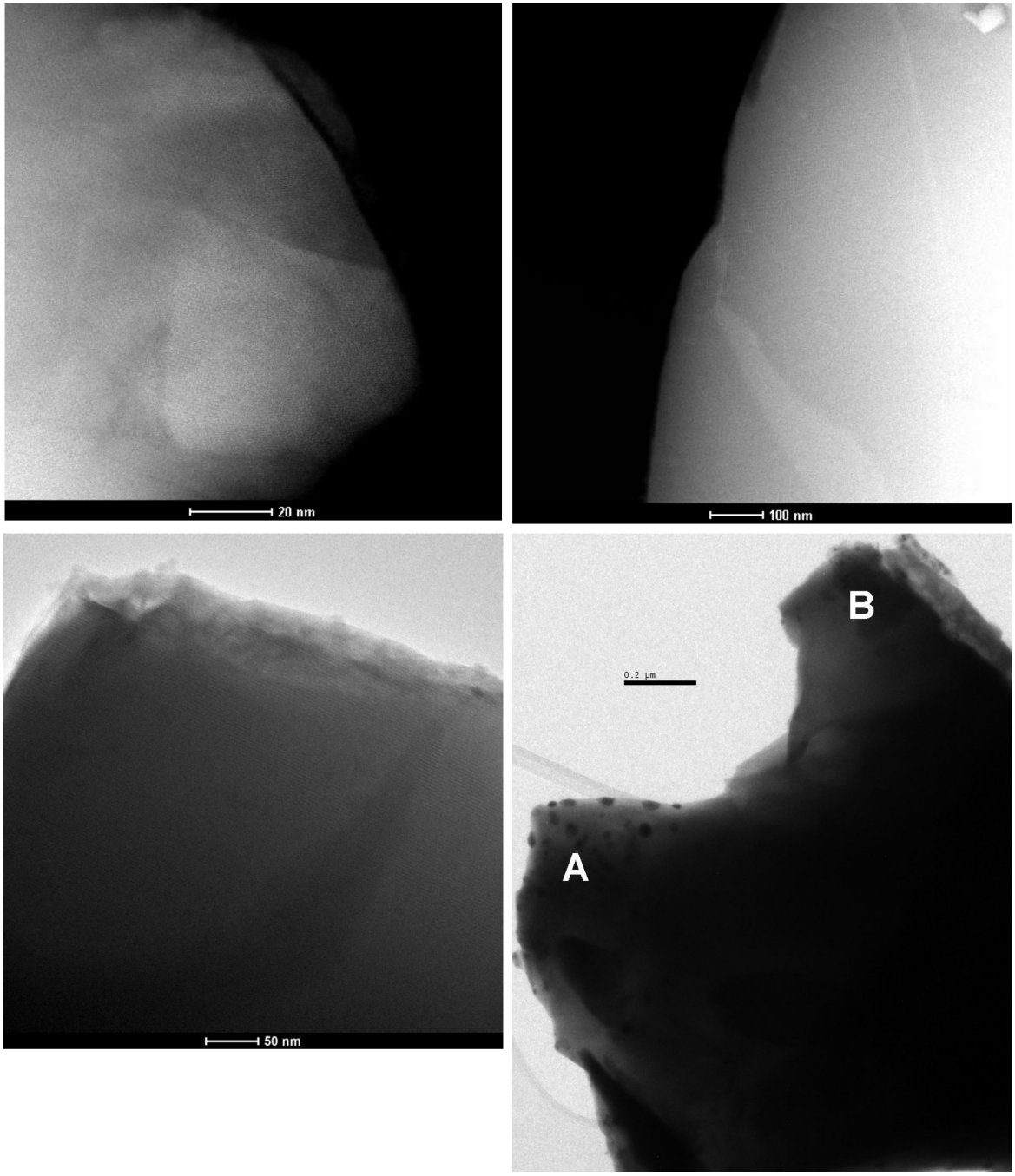

Figure SI 3. Low resolution HAADF-STEM (upper row) and TEM (bottom row) images illustrating average domain size for $Ba_8Au_{16}P_{30}$.