Supplemental Information

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From simple to complex crystal chemistry in the *RE*-Au-*Tt* systems (*RE* = La, Ce, Pr, Nd; *Tt* = Ge, Pb)

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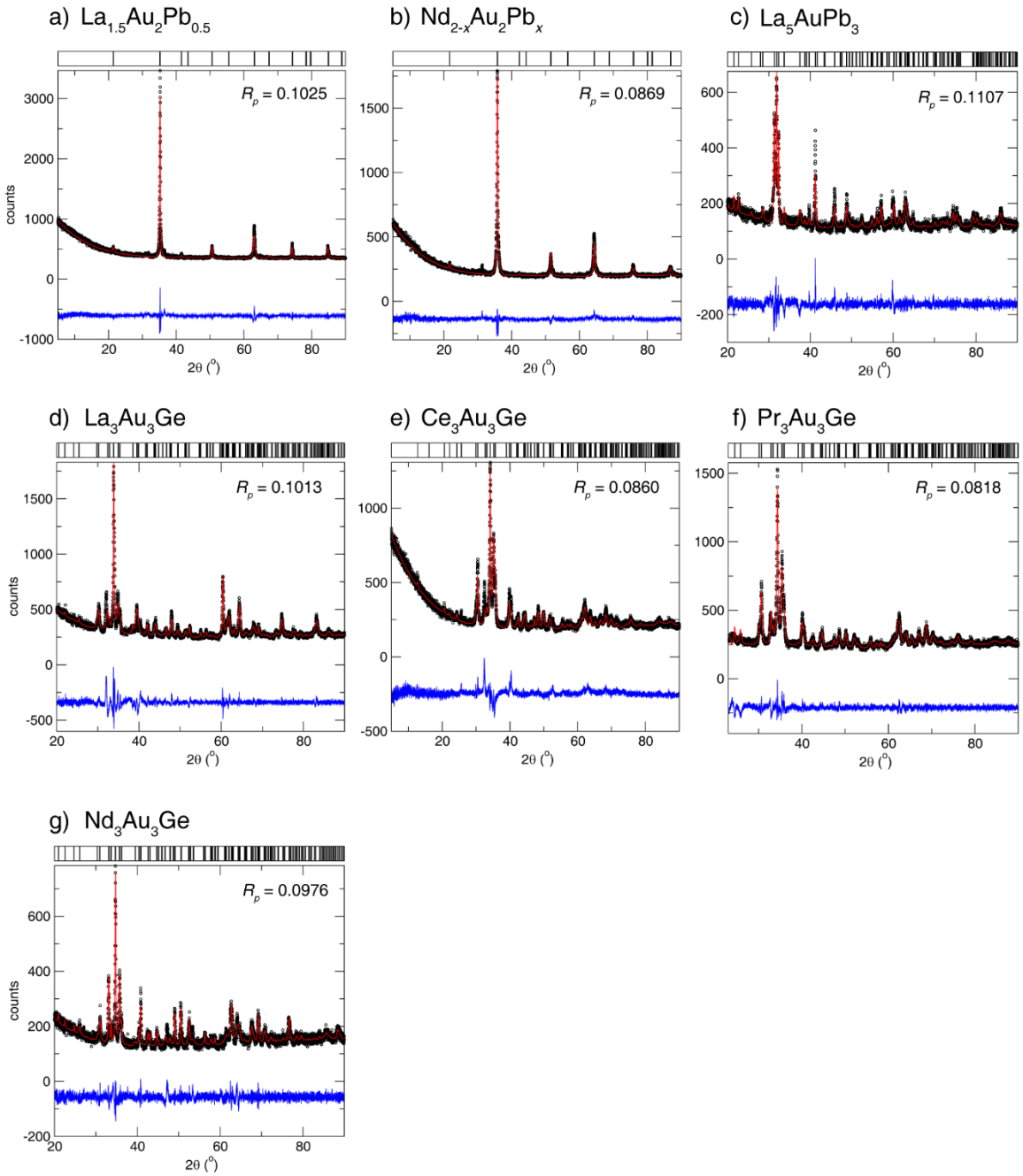

Figure S1. Le Bail refined powder X-ray diffraction patterns for reported *RE*-Au-*Tt* compounds

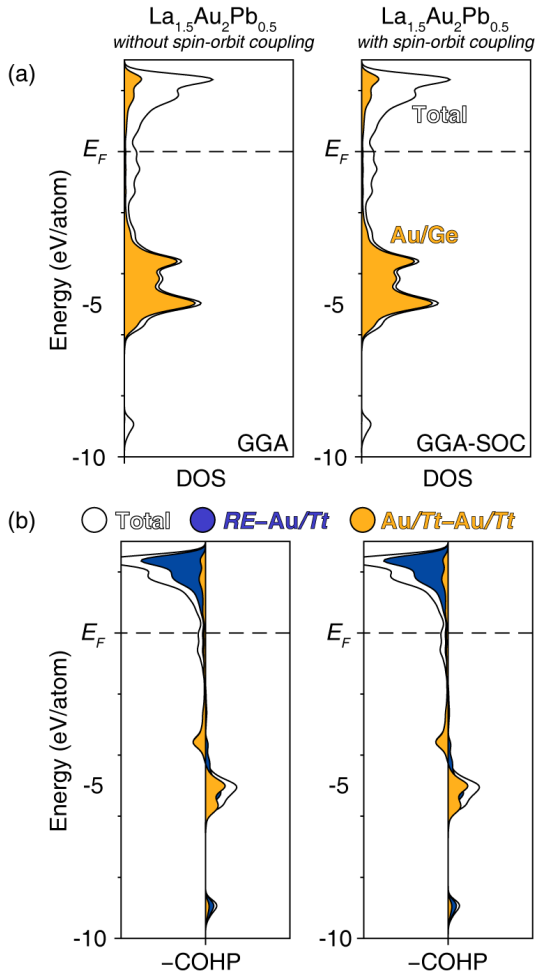

Figure S2. Comparison of spin-orbit and non-spin-orbit coupled (a) DOS and (b) COHP curves for the $La_{1.5}Au_2Pb_{0.5}$ structure. The differences between these curves are minimal, and thus spin-orbit coupling effects do significantly impact these systems.

Table S1. Anisotropic atomic displacement parameters from single crystal diffraction.

Compound	Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
$La_{1.5}AuPb_{0.5}$							
	Au1	0.0212(4)	0.0212(4)	0.0212(4)	0	0	0
	La1	0.0277(6)	0.0277(6)	0.0277(6)	0	0	0
	Pb1	0.0277(6)	0.0277(6)	0.0277(6)	0	0	0
La_5AuPb_3							
	Pb1	0.0181(4)	0.0147(5)	0.0266(5)	0	0	0.0073(2)
	Au1	0.0257(9)	0.0257(9)	0.0415(13)	0	0	0.0129(4)
	La1	0.0199(6)	0.0199(6)	0.0178(8)	0	0	0.0100(3)

	La2	0.0146(7)	0.0206(6)	0.0267(7)	0	0	0.0073(4)
La_3Au_3Ge							
	Au1	0.0189(5)	0.0178(5)	0.0146(5)	0.0014(3)	0.0027(3)	0.0085(4)
	Ge1	0.0189(5)	0.0178(5)	0.0146(5)	0.0014(3)	0.0027(3)	0.0085(4)
	La1	0.0212(7)	0.0272(8)	0.0117(7)	-0.0026(5)	-0.0017(4)	0.0171(6)
	Au2	0.0297(15)	0.0297(15)	0.052(3)	0	0	0.0148(8)
	Ge2	0.0297(15)	0.0297(15)	0.052(3)	0	0	0.0148(8)
	Au3	0.0135(15)	0.0135(15)	0.097(4)	0	0	0.0068(7)
	Ge3	0.0135(15)	0.0135(15)	0.097(4)	0	0	0.0068(7)

Table S2. DFT optimized total energies.

Compound	Energy (eV/atom)
$La_{1.5}AuPb_{0.5}$	-4.98918
La_5AuPb_3	-5.37135
La_3Au_3Ge	-5.45720

Table S3. DFT optimized unit cell parameters.

Compound	*a* = *b* (Å)	*b* (Å)	*c* (Å)	α	β	γ
$La_{1.5}AuPb_{0.5}$	7.13359	7.13359	7.13359	90	90	90
La_5AuPb_3	9.70803	9.70803	6.86837	90	90	120
La_3Au_3Ge	13.97244	13.94458	6.14630	90.0376	90.2033	120.4187

Table S4. DFT optimized atomic positions.

Compound	Atom	*x*	*y*	*z*
$La_{1.5}AuPb_{0.5}$				
	La1	¼	0.252042	¾
	La2	¼	0.747958	¼
	La3	¾	0.747958	¾
	La4	¾	0.252042	¼
	La5	½	0	½
	La6	0	0	0
	Pb1	0	½	½
	Pb2	½	½	0

	Au1	0	0	½
	Au2	½	0	0
	Au3	0	½	0
	Au4	½	½	½
	Au5	¼	0.751889	¾
	Au6	¼	0.248111	¼
	Au7	¾	0.751889	¼
	Au8	¾	0.248111	¾
La_5AuPb_3				
	La1	0.265011	0	¼
	La2	0.734989	0	¾
	La3	0	0.265011	¼
	La4	0	0.734989	¾
	La5	0.734989	0.734989	¾
	La6	0.265011	0.265011	¾
	La7	1/3	2/3	0
	La8	2/3	1/3	0
	La9	2/3	1/3	½
	La10	1/3	2/3	½
	Pb1	0.616751	0	¼
	Pb2	0.383249	0	¾
	Pb3	0	0.616751	¼
	Pb4	0	0.383249	¾
	Pb5	0.383249	0.383249	¼
	Pb6	0.616751	0.616751	¾
	Au1	0	0	0
	Au2	0	0	½
La_3Au_3Ge				
	La1	0.202798	0.040953	0.261032
	La2	0.952469	0.170513	0.278318
	La3	0.839718	0.791697	0.267145
	La4	0.785868	0.953759	0.721503
	La5	0.046269	0.845033	0.739595
	La6	0.167178	0.209193	0.733894
	La7	0.869461	0.377697	0.601670

La8	0.628057	0.491602	0.594465
La9	0.507116	0.127848	0.588229
La10	0.450896	0.285107	0.071252
La11	0.708415	0.160436	0.062233
La12	0.837147	0.549573	0.072114
La13	0.552400	0.708745	0.936956
La14	0.285406	0.835086	0.922179
La15	0.159424	0.450226	0.935135
La16	0.130248	0.624579	0.408804
La17	0.380350	0.498991	0.407358
La18	0.495828	0.874642	0.394744
Ge1	0.061632	0.783268	0.214591
Ge2	0.278376	0.061383	0.787040
Ge3	-0.001879	0.004620	0.498651
Ge4	0.665796	0.332259	0.865948
Ge5	0.668598	0.332130	0.304145
Au1	0.443934	0.054920	0.103241
Au2	0.942201	0.392062	0.121087
Au3	0.611230	0.549826	0.114104
Au4	0.548429	0.935335	0.880252
Au5	0.059527	0.612201	0.890283
Au6	0.389328	0.448033	0.891629
Au7	0.114519	0.392674	0.452627
Au8	0.612722	0.720694	0.451526
Au9	0.276591	0.888809	0.445343
Au10	0.217428	0.279284	0.218835
Au11	0.718860	0.937668	0.208651
Au12	0.779362	0.720277	0.781297
Au13	0.940448	0.221961	0.788289
Au14	0.897705	0.617709	0.554886
Au15	0.388382	0.272569	0.554001
Au16	0.721222	0.109579	0.547127
Au17	0.335487	0.663776	0.148869
Au18	-0.009976	0.008266	0.003727
Au19	0.341030	0.665017	0.677224

Table S5. Calculated Bader charges for $La_{1.5}AuPb_{0.5}$, La_5AuPb_3, and La_3Au_3Ge from density functional theory.

$La_{1.5}AuPb_{0.5}$		La_5AuPb_3		La_3Au_3Ge	
La1	+1.144	La1	+1.239	La1	+1.491
Pb1	+0.072	La2	+0.914	Au*	−1.361
Au1	−0.876	Au	−1.128	Ge*	−1.329
		Pb	−1.472		

*Au and Ge charges were averaged across sites