Supporting Info

Crystal structure and properties of layered pnictides $BaCuSi_2Pn_3$ (*Pn* = P,As)

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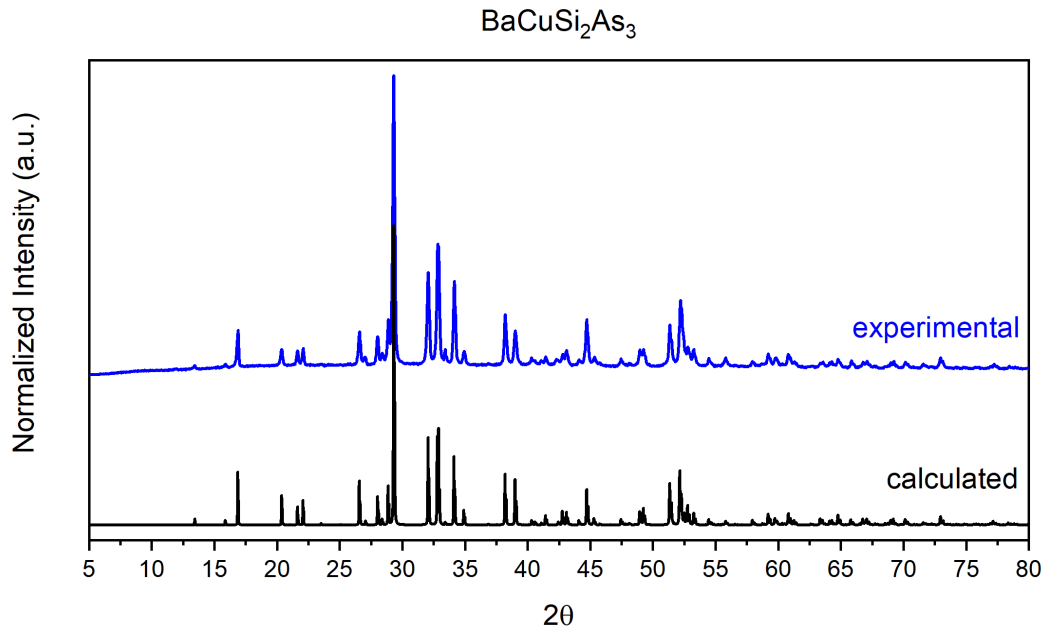
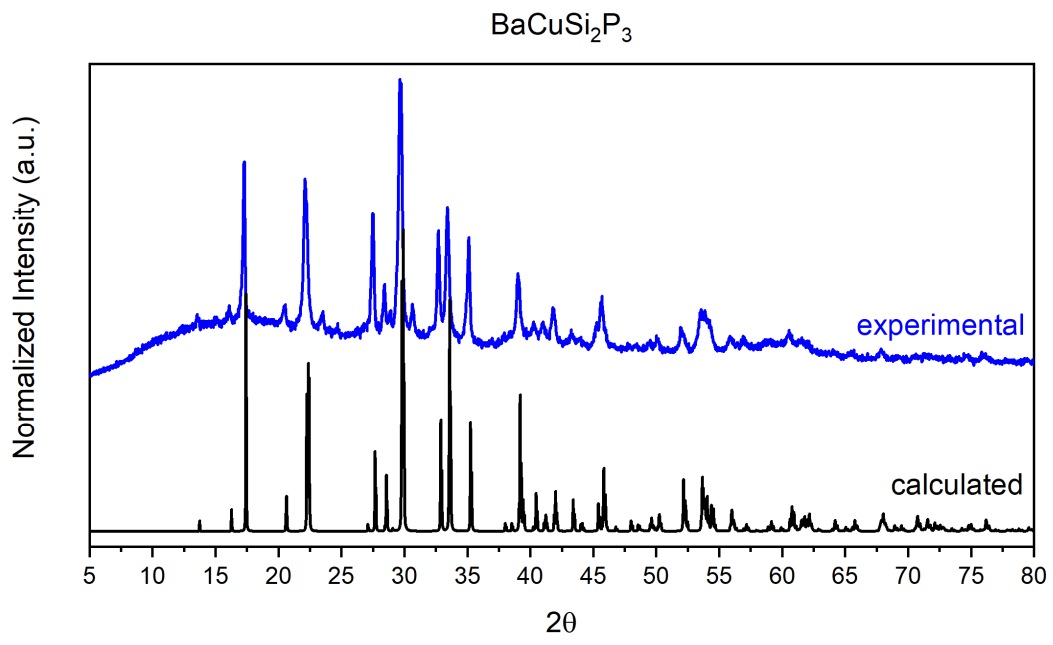
Figure S1



Experimental (blue) and theoretical (black) powder X-ray diffraction patterns for $BaCuSi_2As_3$.

Figure S2



Experimental (blue) and theoretical (black) powder X-ray diffraction patterns for $BaCuSi_2P_3$.

Table S1 *Atomic coordinates and equivalent atomic displacement parameters*

Atom	Wyckoff	x/a	y/b	z/c	Occ.	U_{eq}/Å^2
$BaCuSi_2As_3$						
Ba	4*c*	0.24612(5)	¼	0.9963(2)	1	0.0140(2)
Cu	4*c*	0.9584(1)	¾	0.5741(3)	1	0.0194(4)
Si	8*d*	0.0149(2)	0.5584(2)	0.2103(4)	1	0.0087(5)
As1	4*c*	0.07226(9)	¾	0.9933(2)	1	0.0101(3)
As2	8*d*	0.13572(6)	0.45136(8)	0.5035(2)	1	0.0107(2)
$BaCuSi_2P_3$						
Ba	2*e*	0.71758(6)	¼	0.50290(4)	1	0.00503(8)
Cu	2*e*	0.07842(1)	¾	0.90793(9)	1	0.0068(2)
Si	4*f*	0.2697(2)	0.44200(9)	0.9722(1)	1	0.0047(2)
P1	2*e*	0.4108(3)	¼	0.8648(2)	1	0.0053(2)
P2	4*f*	0.8748(2)	0.55126(8)	0.7394(1)	1	0.0050(2)

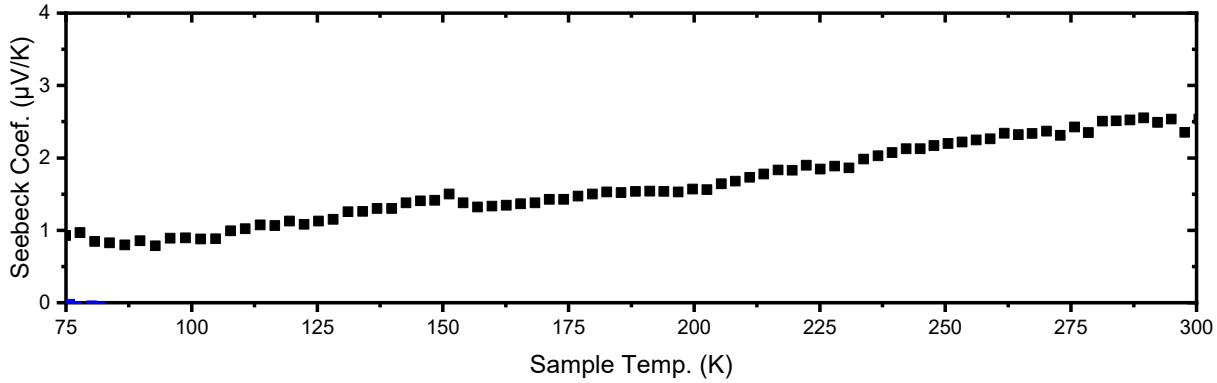
Table S2 *Selected Bond Distances and Bond Angles*

	Distance (Å)		Angle (°)
$BaCuSi_2As_3$			
Ba-As1	3.314(2)	As2-Cu-As2	117.19(8)
Ba-As2	3.429(1)	As1-Cu-As2	114.90(4)
Ba-Cu	3.345(2)	As1-Si-As2	115.5(1)
Cu-As1	2.447(2)	As2-Si-As2	102.79(8)
Cu-As2	2.477(1)	Cu-As1-Si	98.00(7)
Cu-Si	2.725(2)	Si-As2-Si	116.1(1)
Si-Si	2.331(4)	Si-As2-Cu	89.23(7)
Si-As1	2.371(2)		
Si-As2	2.371(2)		
$BaCuSi_2P_3$			
Ba-P1	3.216(2)	P2-Cu-P2	117.95(5)
Ba-P2	3.3438(8)	P1-Cu-P2	118.01(3)
Ba-Cu	3.233(1)	P1-Si-P2	120.24(6)
Cu-P1	2.335(1)	P2-Si-P2	101.57(5)
Cu-P2	2.359(1)	Cu-P1-Si	89.13(4)
Cu-Si	2.805(1)	Si-P2-Si	120.14(9)
Si-Si	2.330(2)	Si-P2-Cu	96.55(4)
Si-P1	2.254(1)		
Si-P2	2.273(1)		

Table S3 *Comparison of unit cell parameters and atom positions from SCXRD experiment and those after full relaxation in VASP for $BaCuSi_2As_3$. For $BaCuSi_2P_3$ only cell volume was relaxed before calculations.*

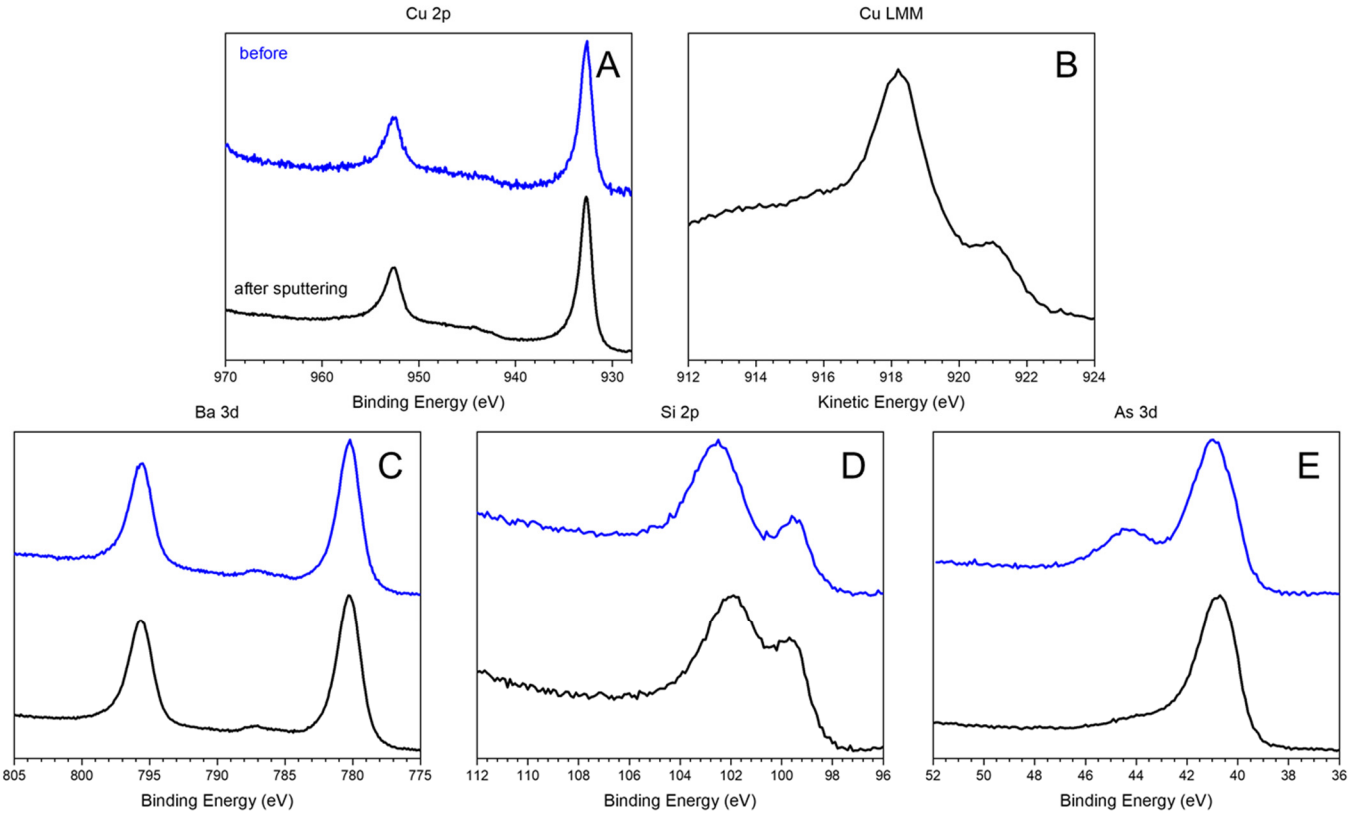
	$BaCuSi_2As_3$ SCXRD	**$BaCuSi_2As_3$ VASP**
a (Å)	13.169(5)	13.112
b (Å)	10.502(3)	10.353
c (Å)	4.6154(1)	4.4817
V (Å^3)	638.3(4)	608.4
Ba1 (x/a, y/b, z/c)	(0.24612, 0.25, 0.99633)	(0.24530, 0.25, 0.99256)
Si1 (x/a, y/b, z/c)	(0.01499, 0.55842, 0.2103)	(0.01562, 0.06113, 0.71234)
Cu1 (x/a, y/b, z/c)	(-0.04153, 0.75, -0.4257)	(-0.03781, 0.75, -0.04269)
As1 (x/a, y/b, z/c)	(0.07226, 0.75, -0.0067)	(0.07325, 0.75, -0.02768)
As2 (x/a, y/b, z/c)	(0.13572, 0.45136, 0.50354)	(0.13805, 0.44915, 0.50146)
	$BaCuSi_2P_3$ SCXRD	**$BaCuSi_2P_3$ VASP**
a (Å)	4.5659(2)	4.5145
b (Å)	10.1726(6)	10.0581
c (Å)	6.8236(4)	6.7468
V (Å^3)	299.10(3)	289.12
β (°)	109.311(2)	109.311

Figure S3



A temperature dependence of the Seebeck coefficient for $BaCuSi_2As_3$ in the range 75-300K. The positive values indicate holes are the main charge carriers and the absolute values are low which is typical for a metal. Data below 75 K become very noisy.

Figure S4



XPS study of $BaCuSi_2As_3$. XP spectra before (blue) and after sputtering (black) for 20s are shown. Cu LMM peak is at 918.0 eV and Cu 2p is at 932.6 eV making the auger parameter 1850.6 eV. Significant improvements were made to the spectra after sputtering for Si 2p and As 3d. The higher energy peaks in Si 2p and As 3d can be described as Si^{4+} and As^{3+} respectively. These species are common in their respective oxides and are most likely surface oxides and not representative of the bulk sample.