

# SUPPORTING INFORMATION

## Blue Phosphorene on Au(111): theory, spectroscopy and diffraction reveal the role of single Au adatoms.

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### Figure S1

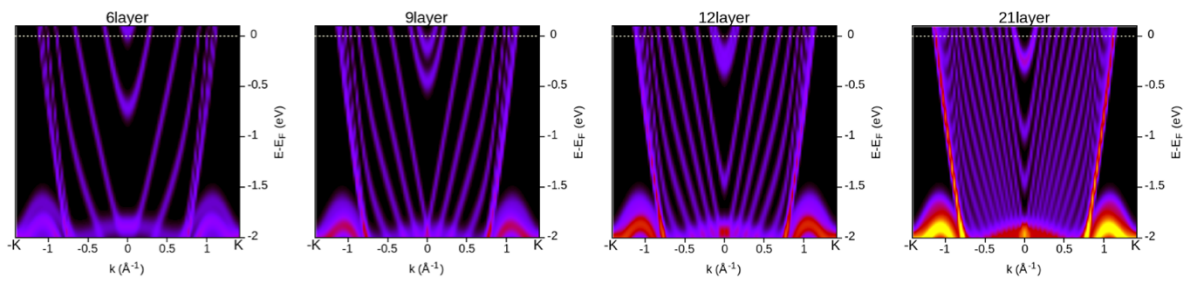
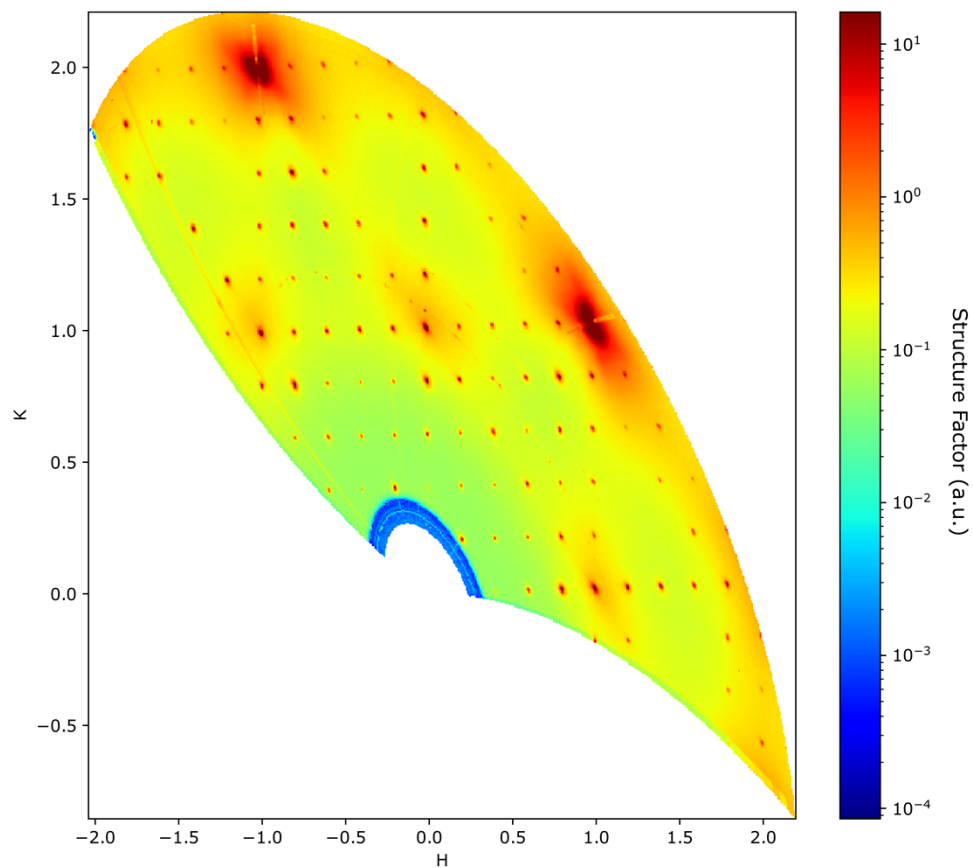


Figure S1 shows the calculated band structure of Au(111) along  $\Gamma$ -K in the reciprocal space as function of electron binding energy for four different slab thickness, 6, 9, 12, and 21 layers. In this binding energy window, 0.0-2.0 eV, the *sp*-bands are dominant, while the stronger Au *d*-band start to appear at the bottom edge. The well-known Shockley surface state of Au(111), located around  $\Gamma$  between Fermi energy and  $\sim 0.5$  eV, becomes evident only for slabs thicker than 12 layers.

**Figure S2**



*Figure S2 shows the in-plane reciprocal space map of SXR D performed on BlueP-Au/Au(111), for fixed diffraction index  $L = 0.10$ .*

Figure S3

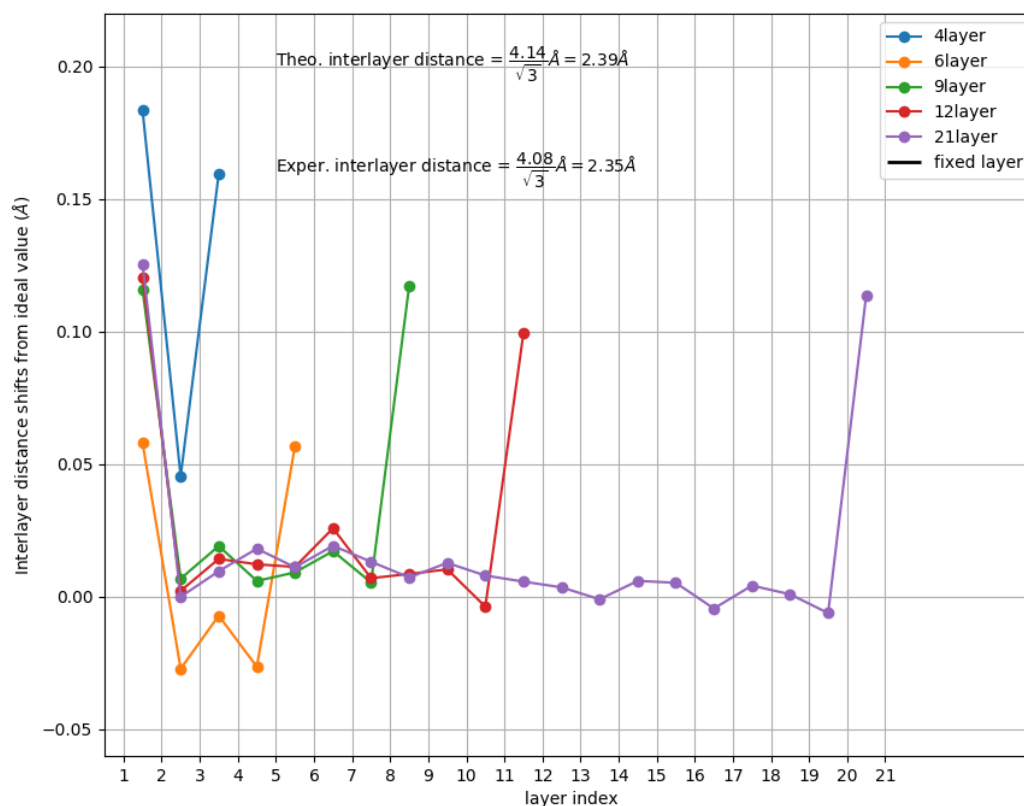


Figure S3 displays the deviations from the ideal value of the distance between atomic planes for different of Au(111) slab thicknesses. The x axis deploys the layer index, i.e. the ordinal number associated with the atomic plane, being 1 the topmost plane. The interplanar distance between  $X^{\text{th}}$  and  $X+1^{\text{th}}$  plane falls between X and X+1 index. Only for slab thicker than 9 layer the interplanar distance between internal planes converges to a constant value. 6-layer slab experiences larger distance variation, although the overall average remains almost unchanged. Conversely, interplanar distances in the 4-layer slab are constantly overestimated, occasionally by more than 0.15 Å.

**Table S1**

Element	X (Å)	Y (Å)	Z (Å)
Au	-5.8439	11.8293	2.3722
Au	-2.9009	11.8405	2.3890
Au	-0.0004	11.8498	2.4055
Au	2.8991	11.8415	2.3887
Au	5.8424	11.8299	2.3722
Au	-0.0012	1.7096	2.3722
Au	2.9462	1.7011	2.3686
Au	5.8766	1.7133	2.4041
Au	8.7701	1.7135	2.4081
Au	11.6992	1.7018	2.3690
Au	-1.4827	4.2530	2.3893
Au	1.4798	4.2528	2.3890
Au	4.4220	4.2327	2.4041
Au	7.3233	4.2281	2.4485
Au	10.2243	4.2328	2.4088
Au	-2.9397	6.7596	2.4102
Au	-0.0015	6.7828	2.4136
Au	2.9382	6.7600	2.4055
Au	5.8690	6.7384	2.4081
Au	8.7778	6.7383	2.4088
Au	-4.3820	9.2747	2.3893
Au	-1.4506	9.2927	2.4136
Au	1.4491	9.2934	2.4091
Au	4.3807	9.2753	2.3887
Au	7.3234	9.2809	2.3690
Au	-4.3466	10.9652	4.7390
Au	-1.4434	10.9702	4.8253
Au	1.4414	10.9695	4.8243
Au	4.3447	10.9652	4.7385
Au	7.3229	10.9939	4.7161
Au	1.4633	0.8448	4.7158
Au	4.4040	0.8650	4.7602
Au	7.3223	0.8636	4.8149
Au	10.2420	0.8648	4.7617
Au	13.1824	0.8448	4.7161
Au	-0.0010	3.4383	4.7390
Au	2.9511	3.3815	4.7602
Au	5.8724	3.3905	4.9034
Au	8.7725	3.3906	4.9054
Au	11.6952	3.3812	4.763

Atomic coordinates (x;y;z) of the unit cell that delivers the best fit with SXRD data.

Au	-1.4563	5.9500	4.8273
Au	1.4549	5.9501	4.8253
Au	4.4092	5.9094	4.8149
Au	7.3226	5.9019	4.9054
Au	10.2362	5.9098	4.8182
Au	-2.8991	8.4490	4.8273
Au	-0.0007	8.4563	4.9025
Au	2.8968	8.4487	4.8243
Au	5.8699	8.4374	4.7617
Au	8.7758	8.4377	4.7623
Au	7.3440	12.7212	7.0095
Au	2.8604	0.0027	7.0288
Au	5.8302	0.0146	7.1280
Au	8.8145	0.0143	7.1277
Au	11.7851	0.0025	7.0292
Au	13.2133	2.4754	7.0299
Au	1.4325	2.4758	7.0288
Au	4.3373	2.5040	7.1366
Au	7.3224	2.5261	7.1679
Au	10.3080	2.5038	7.1378
Au	11.7176	5.0414	7.1300
Au	-0.0010	4.9995	7.1207
Au	2.9277	5.0418	7.1280
Au	5.8489	5.0784	7.1679
Au	8.7964	5.0786	7.1693
Au	10.2248	7.6271	7.1300
Au	-1.4858	7.5990	7.1395
Au	1.4828	7.5991	7.1383
Au	4.4196	7.6265	7.1277
Au	7.3223	7.6750	7.1379
Au	8.7505	10.2052	7.0299
Au	-2.9947	10.1846	7.1207
Au	-0.0015	10.1698	7.1383
Au	2.9920	10.1842	7.1193
Au	5.8948	10.2050	7.0292
P	-0.0013	4.7302	8.8658
P	1.6099	7.5259	8.9964
P	3.2254	10.3190	8.8643
P	-0.0012	10.3165	8.9964
P	-3.2281	10.3190	8.8658
P	-1.6125	7.5258	8.9976
P	1.7404	9.4616	11.2616

P	-0.0010	6.4452	11.2623
P	-1.7425	9.4618	11.2623
P	4.0928	2.3631	8.8864
P	7.3224	2.3658	9.0275
P	10.5519	2.3631	8.8876
P	5.7101	5.1583	9.0276
P	8.9348	5.1584	9.0288
P	7.3224	7.9567	8.8877
P	9.0683	3.2191	11.2898
P	7.3220	6.2438	11.2898
P	5.5759	3.2193	11.2890
Au	2.0784	3.6025	9.4810
Au	3.6587	6.3429	9.7289
Au	5.2417	9.0816	9.4809
Au	12.5664	3.6027	9.4819
Au	-3.6613	6.3429	9.7307
Au	9.4033	9.0813	9.4819
Au	3.1619	12.6838	9.4809
Au	-0.0014	12.6823	9.7288
Au	-3.1648	12.6839	9.4810
Au	0.0000	0.0000	0.0000
Au	-1.4648	2.5370	0.0000
Au	-2.9295	5.0741	0.0000
Au	-4.3943	7.6111	0.0000
Au	-5.8591	10.1482	0.0000
Au	2.9295	0.0000	0.0000
Au	1.4648	2.5370	0.0000
Au	-0.0000	5.0741	0.0000
Au	-1.4648	7.6111	0.0000
Au	-2.9295	10.1482	0.0000
Au	5.8591	0.0000	0.0000
Au	4.3943	2.5370	0.0000
Au	2.9295	5.0741	0.0000
Au	1.4648	7.6111	0.0000
Au	-0.0000	10.1482	0.0000
Au	8.7886	0.0000	0.0000
Au	7.3238	2.5370	0.0000
Au	5.8590	5.0741	0.0000
Au	4.3943	7.6111	0.0000
Au	2.9295	10.1482	0.0000
Au	11.7181	0.0000	0.0000
Au	10.2533	2.5370	0.0000
Au	8.7886	5.0741	0.0000
Au	7.3238	7.6111	0.0000
Au	5.8590	10.1482	0.0000
Au	13.1829	0.8457	-2.3919
Au	11.7181	3.3827	-2.3919
Au	10.2533	5.9198	-2.3919

Au	8.7886	8.4568	-2.3919
Au	7.3238	10.9939	-2.3919
Au	1.4648	0.8457	-2.3919
Au	-0.0000	3.3827	-2.3919
Au	-1.4648	5.9198	-2.3919
Au	-2.9295	8.4568	-2.3919
Au	-4.3943	10.9939	-2.3919
Au	4.3943	0.8457	-2.3919
Au	2.9295	3.3827	-2.3919
Au	1.4648	5.9198	-2.3919
Au	-0.0000	8.4568	-2.3919
Au	-1.4648	10.9939	-2.3919
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Au	8.7886	3.3827	-2.3919
Au	7.3238	5.9198	-2.3919
Au	5.8590	8.4568	-2.3919
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Au	-2.9295	6.7654	-4.7839
Au	-4.3943	9.3025	-4.7839
Au	-5.8591	11.8395	-4.7839
Au	2.9295	1.6914	-4.7839
Au	1.4648	4.2284	-4.7839
Au	0.0000	6.7654	-4.7839
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