Supplementary Material

Determining the atomic coordination number in the structure of β_{12} borophene on Ag(111) via X-ray photoelectron diffraction analysis

Luca Bignardi[1,2], Monica Pozzo[3], Albert Zelenika[1†], Francesco Presel[1‡], Paolo Lacovig[2], Silvano Lizzit[2], Dario Alfè[3,4] and Alessandro Baraldi[1,2*]

[1] Department of Physics, University of Trieste, 34127 Trieste, Italy
[2] Elettra Sincrotrone Trieste, AREA Science Park, 34149 Trieste, Italy
[3] Department of Earth Sciences, University College London, WC1E 6BS London, United Kingdom
[4] Dipartimento di Fisica "Ettore Pancini", Università Federico II, 80126 Napoli, 80126, Italy
[†]Present address: Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark
[‡] Present address: Institute of Physics, Graz University, 8010 Graz, Austria.

(*) Address correspondence to Alessandro Baraldi (alessandro.baraldi@elettra.eu)

S1. Determination of the variance for R_{min}

A confidence interval for the results obtained from the R-factor analysis of the XPD patterns was estimated by using an approach inspired by the common practice in LEED and that has been already used successfully in XPD experiments on other 2D materials [1,2]. The variance of R_{min} is calculated according to the equation $\Delta R_{min} = \sqrt{(2/N)} R_{min}$, where N is the number of well-resolved peaks included in the whole data set [3]. In our case we have N=400. Consequently, having $R_{min} = 0.195$ and 0.179 for peak B1 and B3 respectively, we find ΔR_{min}=0.014 for the pattern stemming from component B1, and ΔR_{min}=0.013 for the pattern resulting from B3.

S2. Cluster used in XPD patterns simulations

The borophene structure used as input for the XPD patterns simulations through EDAC stems directly from DFT calculations and it is composed by a total of 75 B atoms. The cluster chosen for the EDAC simulation was a parabolical cluster, with surface mode ON, with maximum radius of 5 Å around the emitter; therefore, we include approximately 30 B atoms around the emitter in the calculation of the XPD pattern. The Ag(111) substrate was not included in the simulations of the XPD patterns.

S3. Supplementary Figure

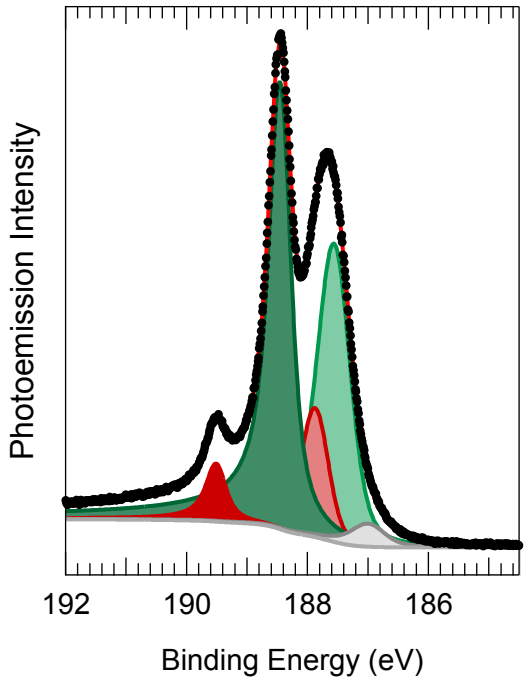

Figure S1. B 1s core level acquired on the borophene layer obtained depositing B in UHV with the Ag(111) substrate temperature at 730 K.

S4. B atomic coordinates for the β_{12} phase on Ag(111)

Coordinates given in Å. The values reported in the last column (z) correspond to the distance of each B atom with the first atomic layer of the Ag surface.

	x	y	z
B	-0.005428	-0.015848	2.441457
B	3.056189	-0.021629	2.358607
B	6.122080	-0.018486	2.356523
B	9.186045	-0.017874	2.355043
B	12.251668	-0.021299	2.359023
B	1.524656	2.496009	2.358439
B	4.589767	2.491564	2.316011
B	7.653789	2.488098	2.339563
B	10.716371	2.492321	2.312450
B	13.782320	2.497019	2.358383
B	-0.003814	4.891586	2.421205
B	3.059639	4.896162	2.408095
B	6.116618	4.890193	2.328081
B	9.189231	4.890065	2.334337
B	12.247902	4.895601	2.414808
B	1.528533	7.408168	2.351986
B	4.590859	7.404439	2.317593
B	7.653234	7.400447	2.312769
B	10.716092	7.404391	2.330848
B	13.778773	7.407871	2.356804
B	-0.003955	9.807768	2.391169
B	3.058224	9.808780	2.433085
B	6.126925	9.806189	2.339118
B	9.182738	9.805574	2.353086
B	12.250875	9.808757	2.435061
B	1.530330	12.322137	2.329576
B	4.590407	12.318112	2.342356
B	7.655568	12.312797	2.279563
B	10.719101	12.317910	2.343120
B	13.777752	12.322127	2.328898
B	1.524201	0.778940	2.353280
B	4.590381	0.781294	2.306503
B	7.653948	0.782817	2.347600
B	10.716216	0.781516	2.301982
B	13.782864	0.779375	2.352328
B	3.058202	3.293772	2.371490
B	6.118943	3.289568	2.360320
B	9.188272	3.288854	2.356780
B	12.248853	3.294460	2.374072
B	-0.005086	3.291389	2.464179
B	1.527868	5.691247	2.349411
B	4.589327	5.694096	2.330320
B	7.653109	5.696420	2.278182
B	10.716583	5.694119	2.341079
B	13.780472	5.690882	2.354704

B	3.057865	8.207907	2.412307
B	6.127286	8.204379	2.347963
B	9.180215	8.203217	2.360322
B	12.249689	8.206858	2.419279
B	-0.004793	8.205318	2.416262
B	1.530695	10.604855	2.346830
B	4.591822	10.607366	2.334860
B	7.655160	10.608163	2.304868
B	10.718523	10.606462	2.340527
B	13.778698	10.604708	2.346819
B	3.058810	13.116978	2.419739
B	6.122478	13.119496	2.325317
B	9.189738	13.119310	2.331404
B	12.248629	13.116528	2.417457
B	-0.004421	13.122162	2.361209
B	-0.005450	1.637221	2.504879
B	3.046835	1.637725	2.443469
B	6.120574	1.635680	2.479204
B	9.187218	1.635744	2.478049
B	12.259227	1.638398	2.437935
B	-0.004303	6.548380	2.468190
B	3.049139	6.550995	2.463133
B	6.114261	6.546774	2.453262
B	9.193521	6.545621	2.457809
B	12.257989	6.551708	2.471049
B	-0.003931	11.463944	2.442719
B	3.050416	11.463147	2.486312
B	6.112269	11.463181	2.447747
B	9.197245	11.462682	2.446521
B	12.258209	11.463675	2.488237

References

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[3] J.B. Pendry, Reliability factors for LEED calculations, J. Phys. C: Solid State Phys. 13 (1980) 937.