Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information: Investigating the Mechanism of Phosphorene Nanoribbon Synthesis by Discharging Black Phosphorus Intercalation Compounds

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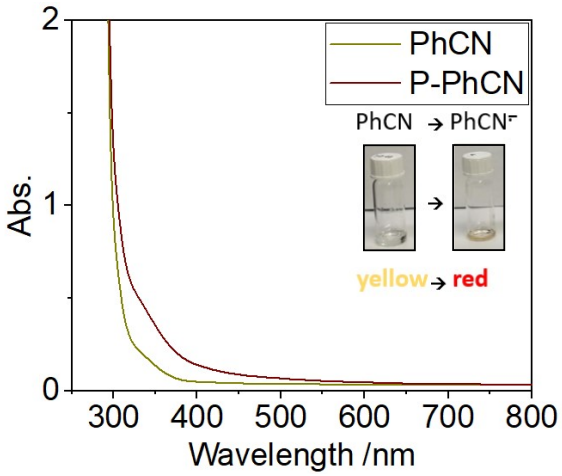
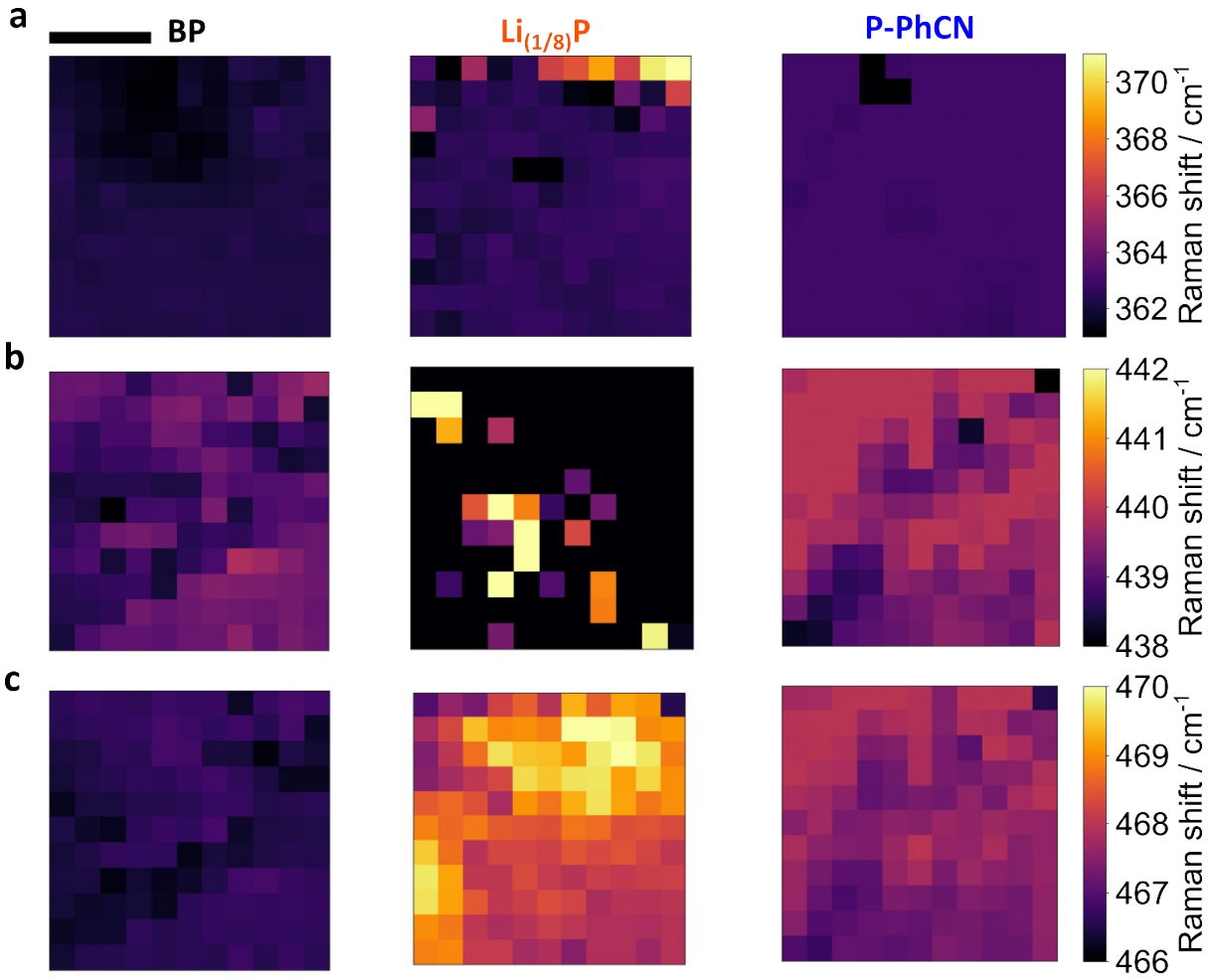
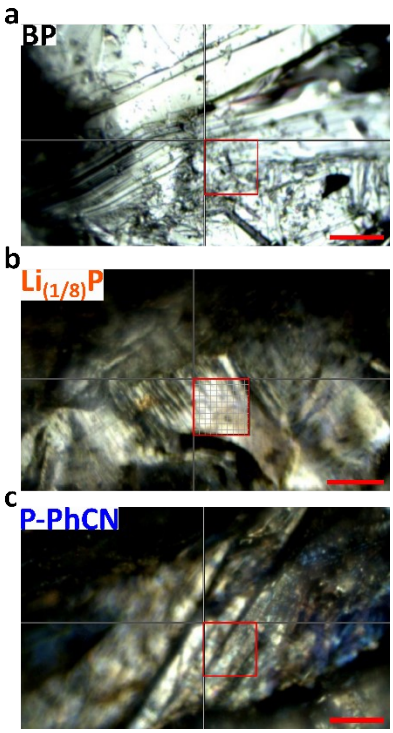


Supplementary figure S1. UV-vis spectra of PhCN before and after addition to $Li_{(1/8)}P$, with photos of PhCN in cuvette before and after addition to $Li_{(1/8)}P$ inset.



Supplementary figure S2. Supplementary Raman map analysis. Fitted centres of Raman peaks arising from (a) A_g^1, (b) B_{2g}, (c) A_g^2 modes in BP, $Li_{(1/8)}P$, and P-PhCN samples. Lateral scale bar = 20 μm.



Supplementary figure S3. Optical micrographs of the (a) BP, (b) $Li_{(1/8)}P$, and (c) P-PhCN samples captured through a through a ×20 objective lens. The crosshairs (white) and 50 μm × 50 μm area used for Raman spectroscopic map analysis (red box) are shown. Scalebar = 50 μm.

Supplementary table S1. The mean intensities, peak centres, and FWHM extracted from the Raman spectroscopy map analysis. The corresponding first standard deviations from the mean are also given.

BP

Peak	*Parameter*	*mean (μ)*	*standard deviation (σ)*
A_g^1	centre	362.0	0.3
	FWHM	3.1	0.2
	intensity	1730	420
B_{2g}	centre	439.0	0.3
	FWHM	3.7	0.5
	intensity	1520	380
A_g^2	centre	466.5	0.2
	FWHM	3.0	0.1
	intensity	2630	940

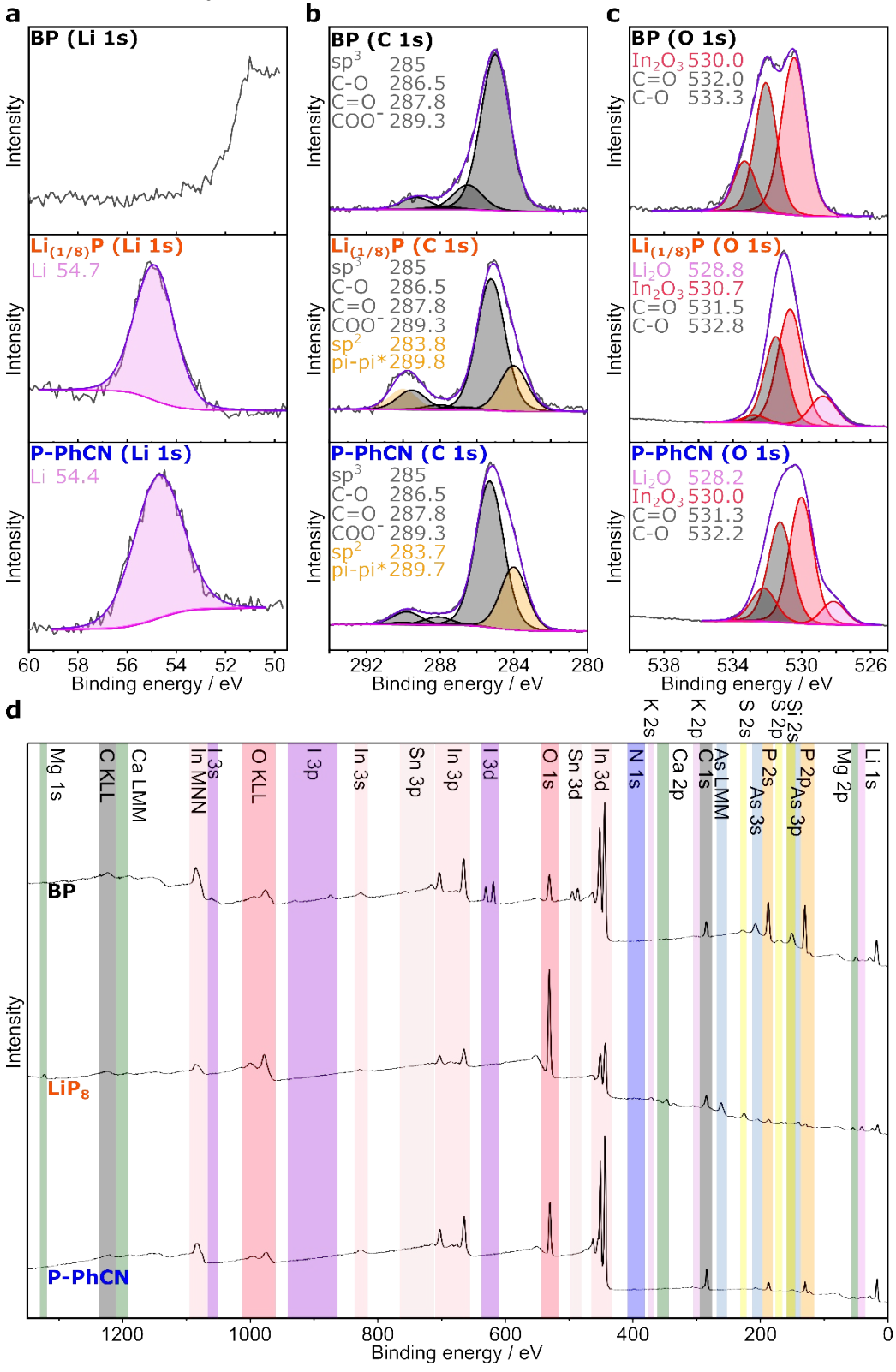
$Li_{(1/8)}P$

Peak	*Parameter*	*mean (μ)*	*standard deviation (σ)*
A_g^1	centre	362.9	1.3
	FWHM	10.1	10.1
	intensity	300	230
B_{2g}	centre	440.8	0.4
	FWHM	9.0	4.4
	intensity	490	240
A_g^2	centre	468.5	0.7
	FWHM	7.8	2.2
	intensity	1020	490

P-PhCN

Peak	*Parameter*	*mean (μ)*	*standard deviation (σ)*
A_g^1	centre	363.0	0.1
	FWHM	5.6	1.1
	intensity	1390	490
B_{2g}	centre	439.6	0.5
	FWHM	6.7	1.6
	intensity	2050	500
A_g^2	centre	467.5	0.3
	FWHM	5.3	0.8
	intensity	4470	1180

XPS further analysis



Supplementary figure S4. High resolution X-ray photoelectron spectroscopy (XPS) lithium 1s, carbon 1s, and oxygen 1s spectra fitted with several components is shown along with the survey spectrum for each samples BP, $Li_{(1/8)}P$, and P-PhCN.

Supplementary table S2. Surface atomic composition extracted from the XPS spectra of BP, $Li_{(1/8)}P$, and P-PhCN.

BP

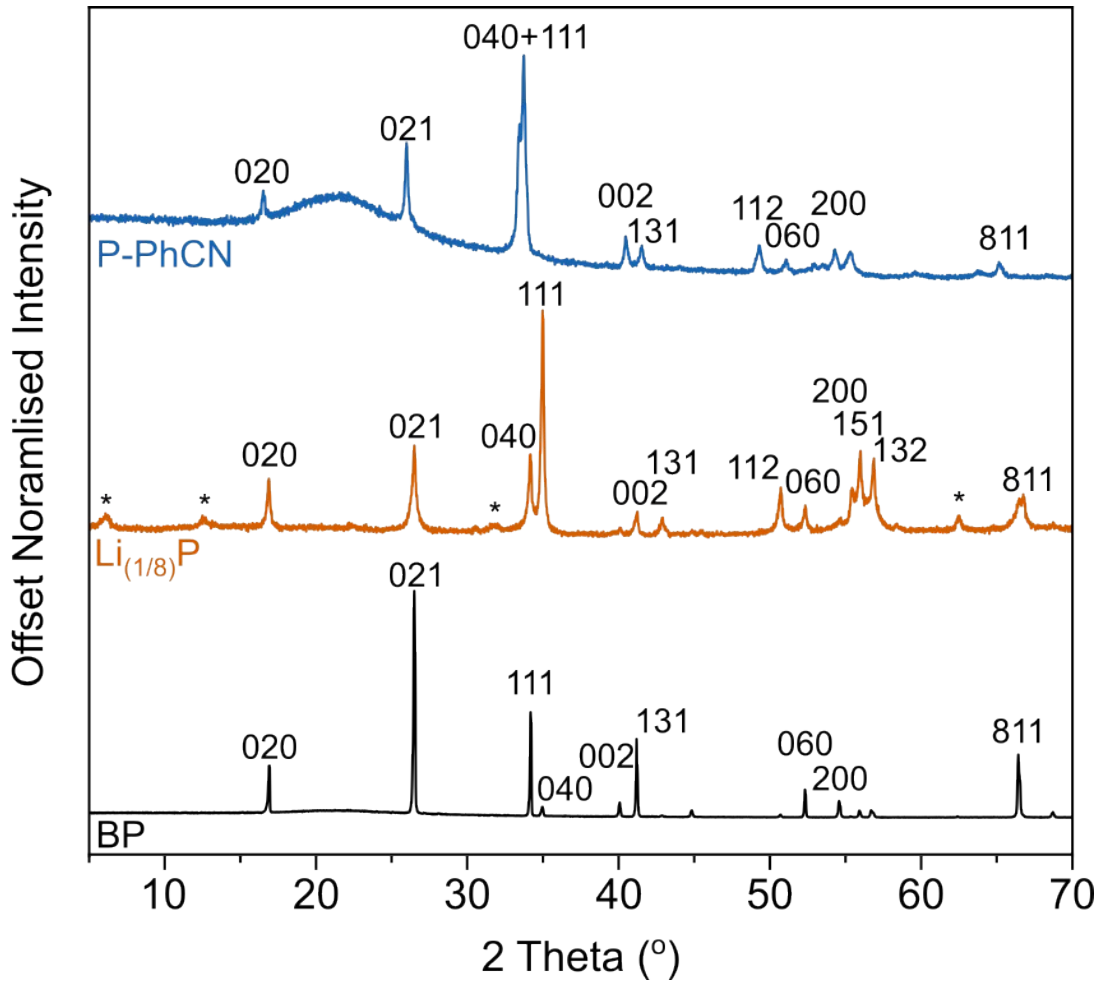
Element	*%*	*Ratio vs P*
C	26.76	0.52
Li	0.00	0.00
O	21.57	0.42
P	51.67	1.00

$Li_{(1/8)}P$

Element	*%*	*Ratio vs P*	*Ratio vs Li*
C	14.43	2.60	0.40
Li	35.99	6.49	1.00
O	44.04	7.94	1.22
P	5.54	1.00	0.15

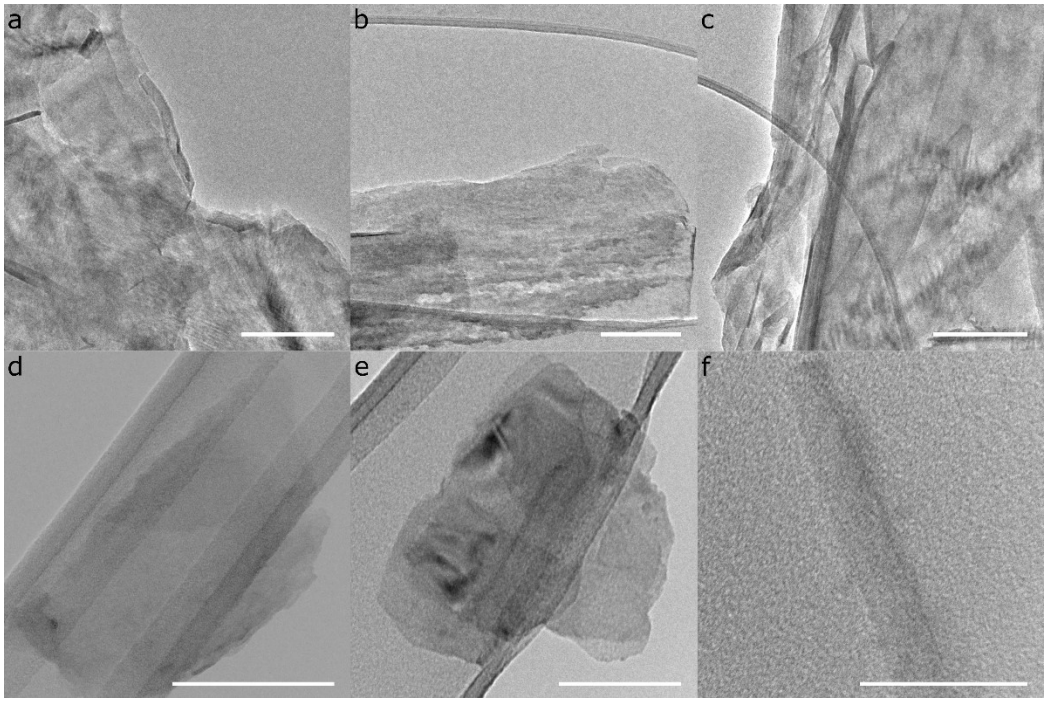
P-PhCN

Element	*%*	*Ratio vs P*	*Ratio vs Li*
C	28.25	2.53	1.05
Li	26.94	2.41	1.00
O	33.64	3.01	1.25
P	11.17	1.00	0.41

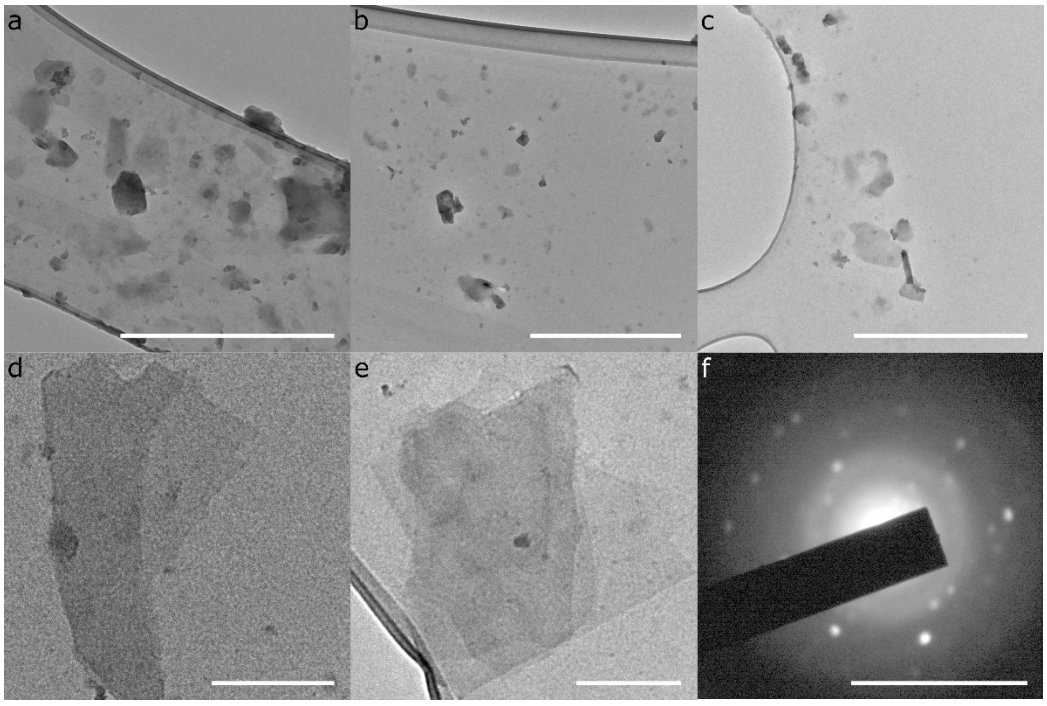


Supplementary Figure 5. Powder xray diffraction (Cu kα) of, from bottom to top, BP, $Li_{(1/8)}P$, and P-PhCN

TEM further analysis

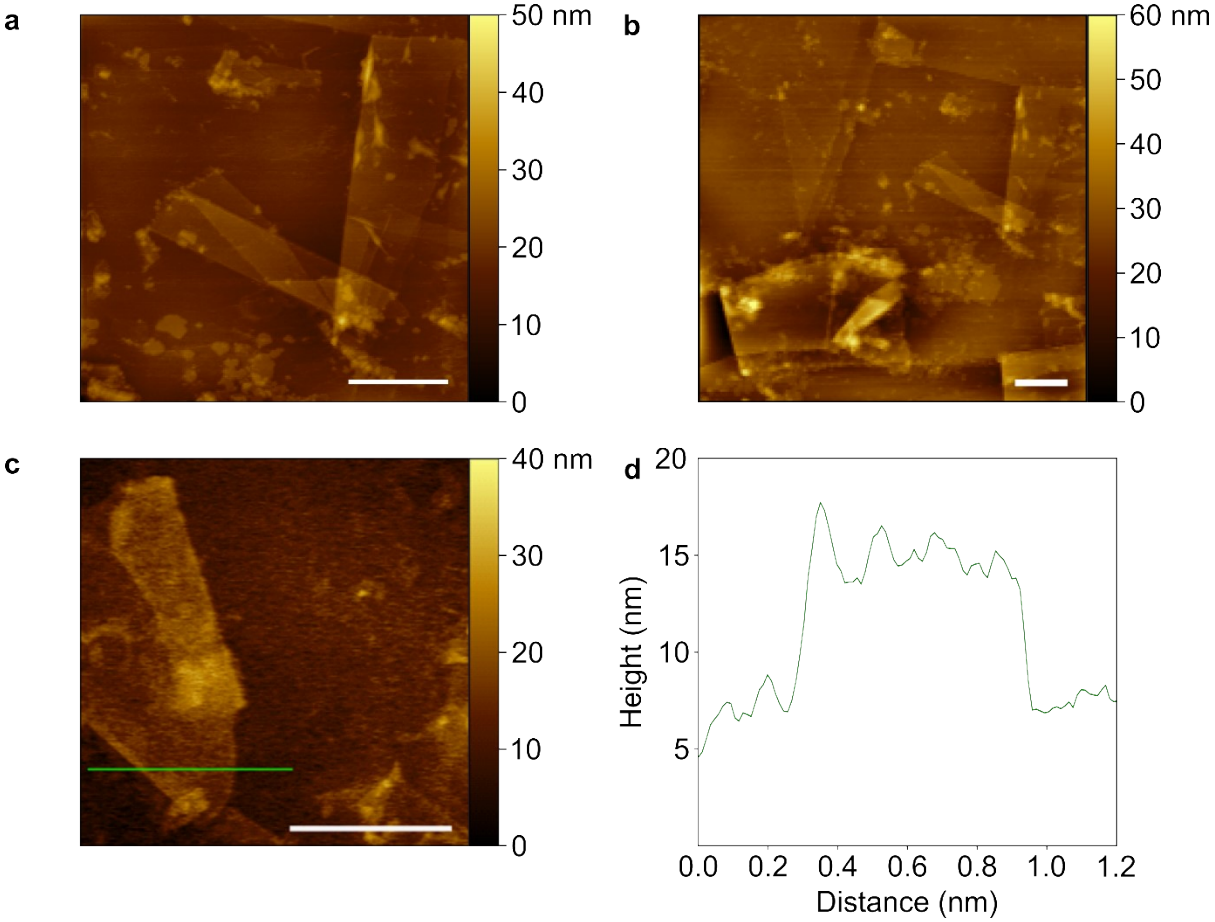


Supplementary figure S6. Additional TEM micrographs of P-PhCN sonicated in NMP. Scalebars: (a-c) = 200 nm, (d,e) = 100 nm, (f) = 50 nm.

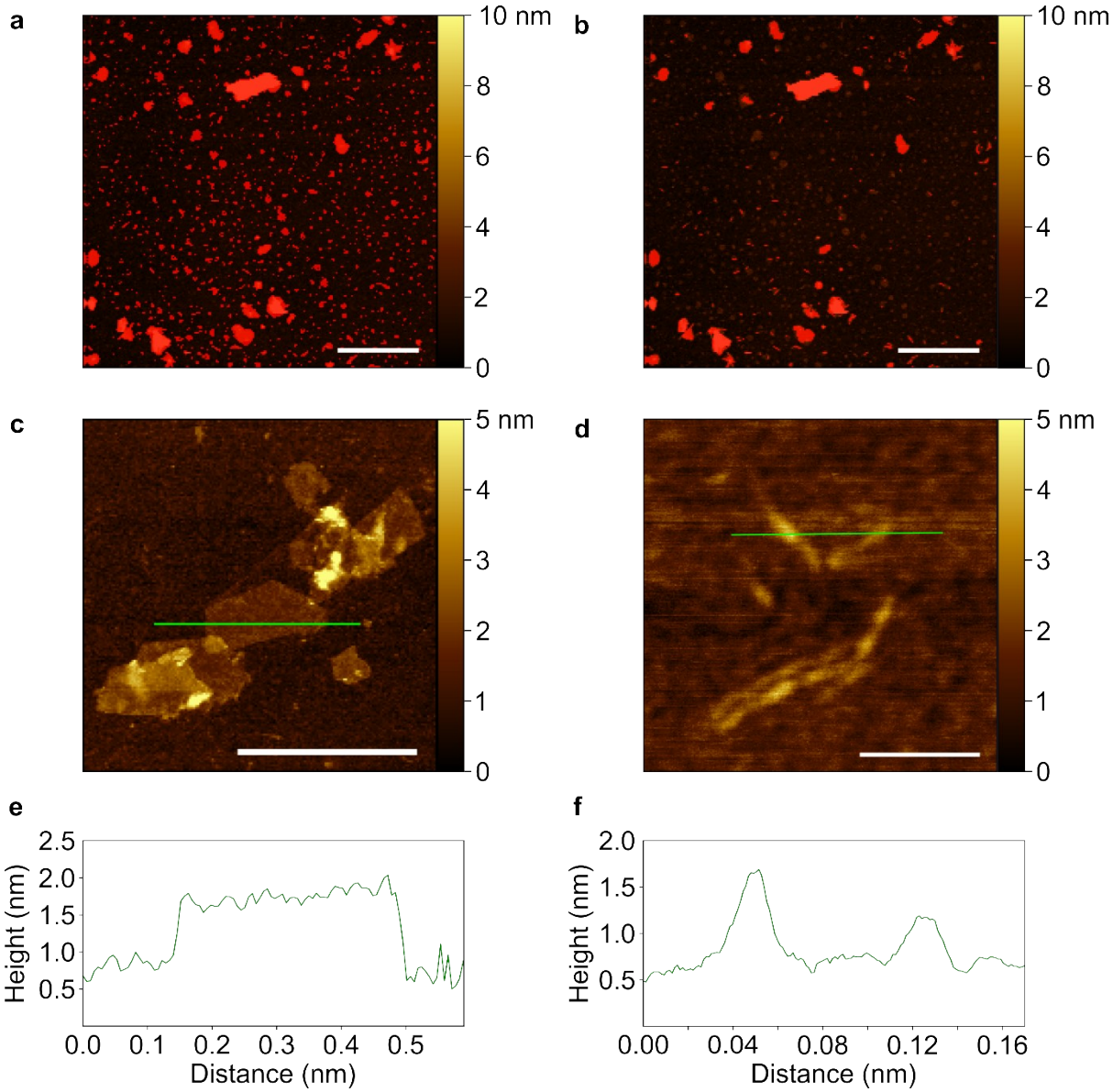


Supplementary figure S7.TEM characterisation of BP sonicated in NMP. (a-e) TEM micrographs of exfoliated BP. Scalebars: (a-c) = 1 μm, (d,e) = 200 nm. (f) 20 nm^{-1}.

AFM further analysis



Supplementary figure S8. AFM images of tape-exfoliated (a,b) BP and (c) $Li_{(1/8)}P$. All scalebars = 1 µm. (d) Height line-profile of $Li_{(1/8)}P$ indicated by green line in c.



Supplementary figure S9. Further analysis of AFM characterisation of tape exfoliated P-PhCN. Data processed AFM image after masking, showing all pixels filtered by a height threshold of (a) 2 nm and (b) 4 nm highlighted in red. (c) AFM image (replot of Main Text Figure 5b) with green line corresponding to height line-profile plotted in (e). (d) AFM image (replot of Main Text Figure 5d) with green line corresponding to height line-profile plotted in (f). Scalebars: (a,b) = 1 μm, (c) = 500 nm, and (d) = 100nm.

Supplementary computational data.

Supplementary Table 3. Energy values from DFT calculations. E refers to output ground state energy from calculation. ΔH_f normalised to unit cell (i.e., output energy), P atom (i.e. output divided by 32) and Li atom (divided by number of lithium per unit cell) * Calculated from $Li^+_{(g)}$ calculation by incorporation of lithium's 1st ionisation energy (0.1980789 Hartree). ‡ Calculated from $Li^0_{(g)}$ value by incorporation of lithium's cohesion energy (0.0738661 Hartree).

	E		ΔH_f		
	Hartree	kJ/mol	kJ mol(unit cell)$^{-1}$	kJ mol(P)$^{-1}$	kJ mol(Li)$^{-1}$
bP	-1.365×10^3	-3.585×10^6			
P_{32}	-1.092×10^4	-2.868×10^7			
$Li^+_{(g)}$	-7.279	-1.911×10^4	-		
$Li^0_{(g)}$ *	-7.477	-1.963×10^4	-		
$Li^0_{(s)}$ ‡	-7.551	-1.982×10^4			
Li_1P_{32}	-1.093×10^4	-2.870×10^7	-65.4	-2.0	-65.4
Li_2P_{32} (Li different)	-1.094×10^4	-2.872×10^7	-164.5	-5.1	-82.2
Li_2P_{32} (Li same)	-1.094×10^4	-2.872×10^7	-176.4	-5.5	-88.2
Li_4P_{32} ("Even")	-1.095×10^4	-2.876×10^7	-350.4	-10.9	-87.6
Li_4P_{32} ("Top")	-1.095×10^4	-2.876×10^7	-179.0	-5.6	-44.8
Li_4P_{32} ("Bottom")	-1.095×10^4	-2.876×10^7	-380.0	-11.9	-95.0
Li_4P_{32} ("Left")	-1.095×10^4	-2.876×10^7	-294.2	-9.2	-73.5
Li_4P_{32} ("Right")	-1.095×10^4	-2.876×10^7	-326.1	-10.2	-81.5
Li_8P_{32}	-1.098×10^4	-2.884×10^7	-849.8	-26.6	-106.2

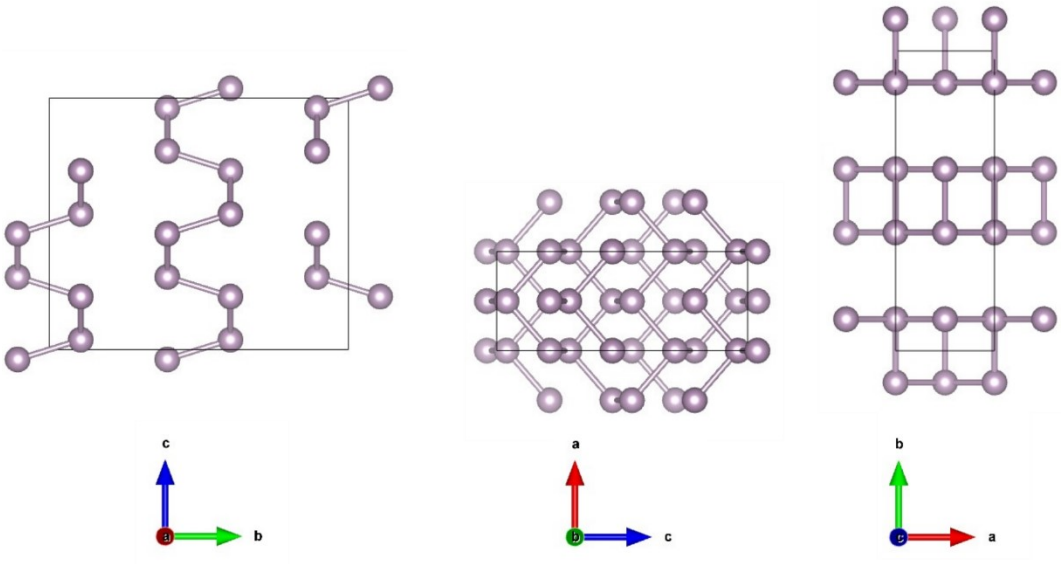
Supplementary Discussion of $Li_{(1/8)}P$ Li Configurations

In the Li_2P_{32} (i.e., $Li_{(1/16)}P$) model, there are two primary configurations for Li placement – same layer vs different layer – as discussed in the main text. However, the different initial configurations are possible for all stoichiometries. Using the P_{32} (2 × 1 × 2) initial supercell, there is only one viable initial configuration each for LiP_{32} and Li_8P_{32}, however, a large number are possible for Li_4P_{32}. The primary configuration (as discussed in the main text) involved placing two Li in each interlayer gallery to maximise Li distribution (here named "Even"). To better represent the potential diversity in $Li_{(1/8)}P$ structures and model systems with more compact Li distributions, a range of Li_4P_{32} input models were created by removing four Li from the relaxed Li_8P_{32} model.

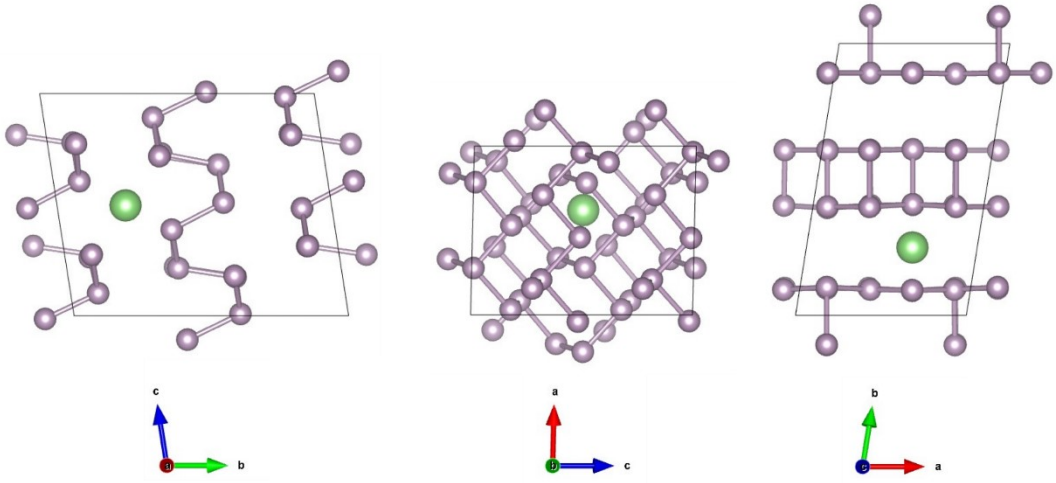
The Li_8P_{32} system showed breakage of several P bonds and a significant distortion of the P framework (Supplementary figure 15, Main text Fig 2i), meaning removal of different selection of Li would provide a fuller understanding of feasible Li_4P_{32} final structures. In this vein, we conceptually cut halfway down the b/c-axes and removed the lithium either side. Cutting the b-axis gave lithium in the *Top* and *Bottom*, restricted to a single interlayer gallery, similar to the "Li_2P_{32} (Li same)" model.

Conversely, cutting down the c-axis gave lithium restricted to the *Left* and *Right* of the cell (Supplementary figure 16).

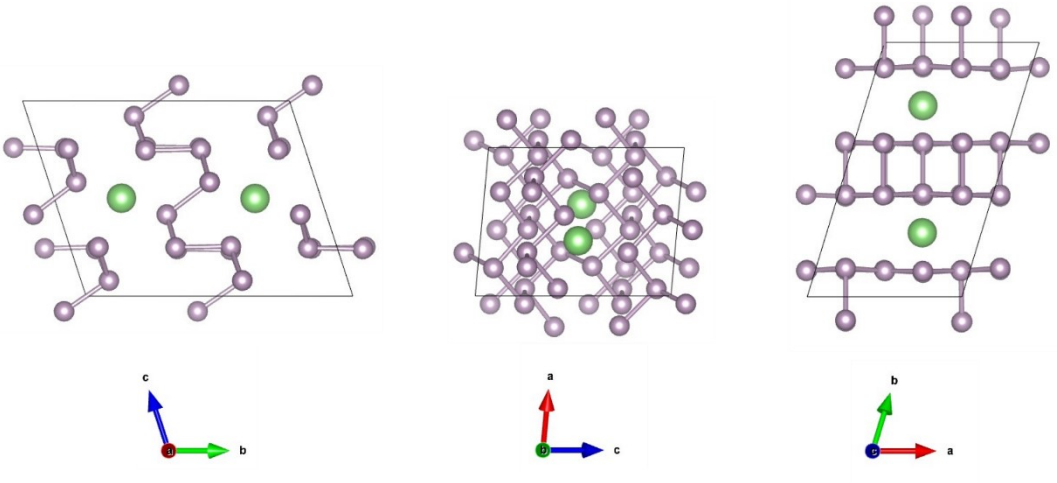
In the *Top* model, where all 4 lithium remain near the intralayer P-P fractures, the fractures are also seen, while all three other models (*Bottom*/*Left*/*Right*) do not show bond cleavage, akin to *Even*. The enthalpy of formation (Supplementary table 3) of *Top* is likewise distinct (-5.6 kJ mol(P)$^{-1}$) from the other four Li_4P_{32} models which all very similar in energy (-9.2 to -11.9 kJ mol(P)$^{-1}$) independent of local Li configuration. The interlayer structure is similar between all Li_4P_{32} structures, where all models show layer-shear to an AB structure with lithium pockets. Given the stacking similarities, the lesser enthalpy of formation for the *Top* model can be attributed to the necessary energy cost of breaking the intralayer P-P bonds. We note that while P-P bond cleavage is less favourable, the energy cost is low (~5.5 kJ mol^{-1}). Taken together, the similarities in energy (both for local Li arrangements and with/without P-P cleavage) and in P-framework stacking further support the concept that there will be limited thermodynamic driven local ordering, and intercalation will likely be highly locally heterogeneous.



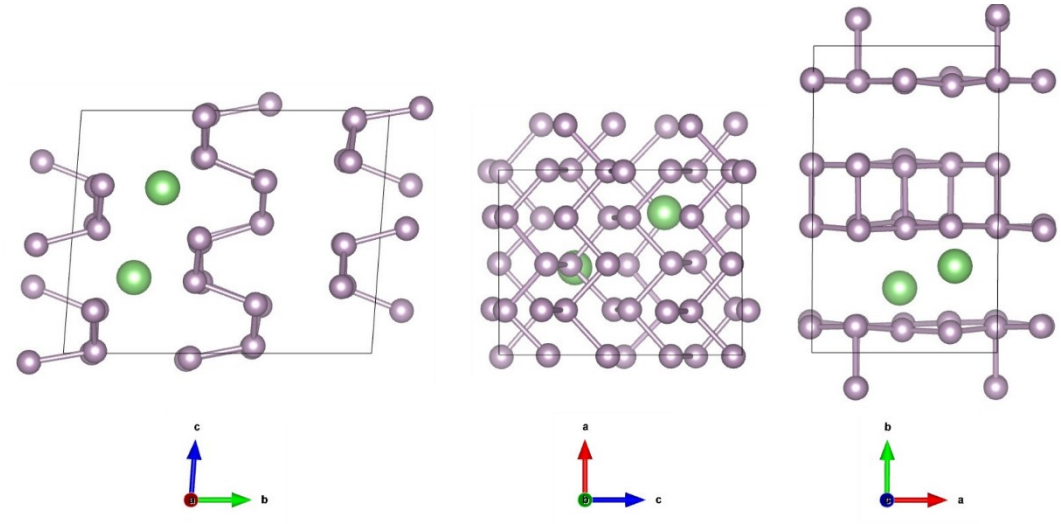
Supplementary figure S10. BP supercell down the (from left to right) a, b, and c axes.



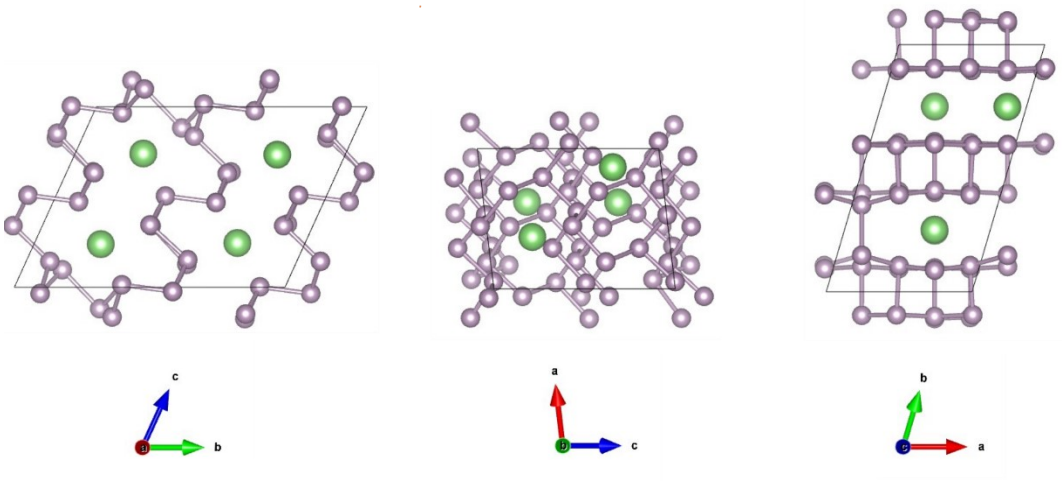
Supplementary figure S11. LiP_{32} supercell down the (from left to right) a, b, and c axes.



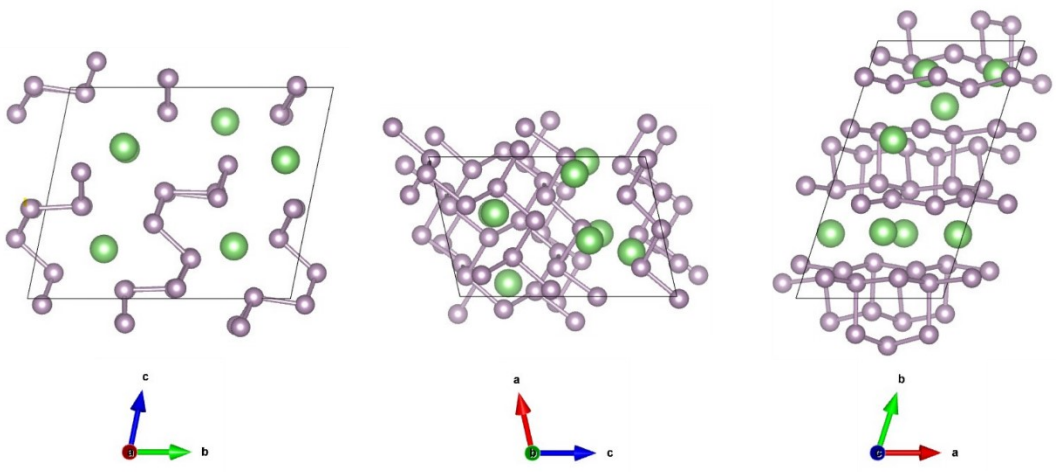
Supplementary figure S12. Li_2P_{32} supercell with Li evenly distributed between interlayer galleries, visualised down the (from left to right) a, b, and c axes.



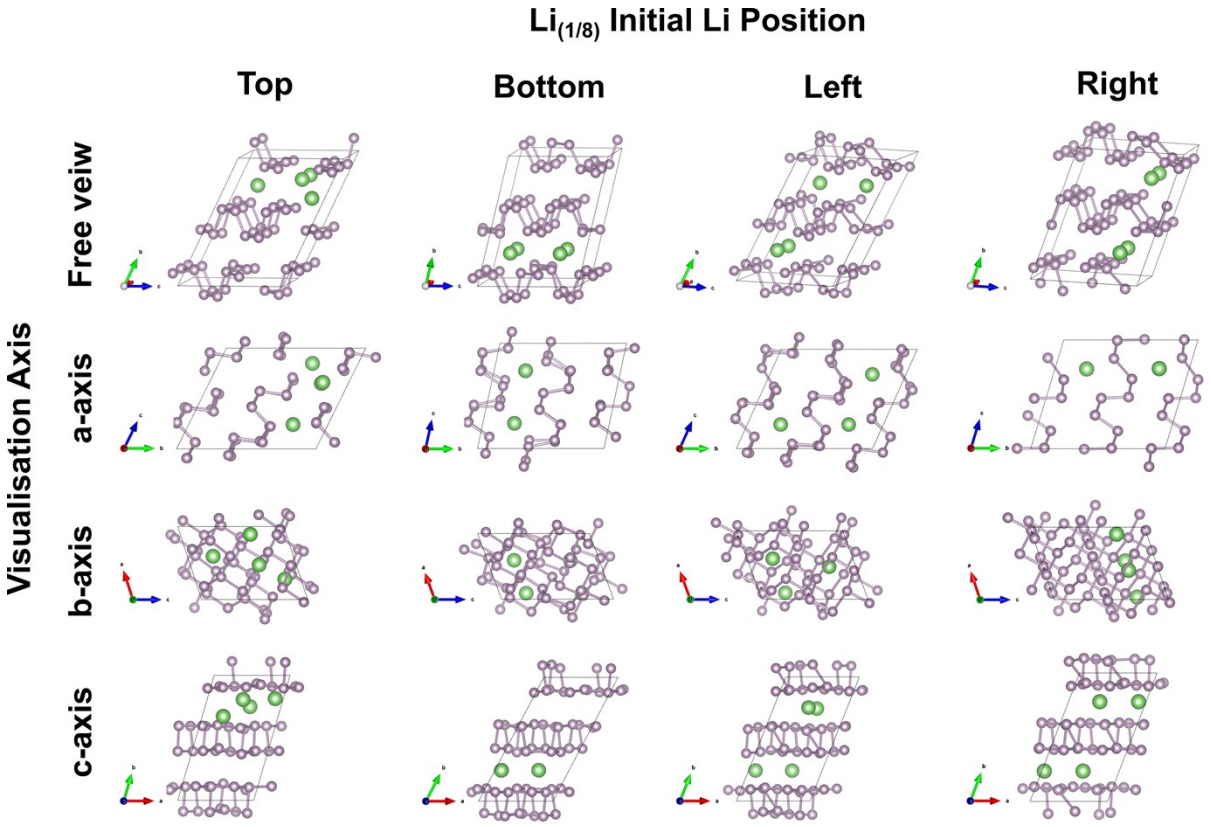
Supplementary figure S13. Li_2P_{32} supercell with both Li in the same interlayer gallery, visualised down the (from left to right) a, b, and c axes.



Supplementary figure S14. Li_4P_{32} supercell visualised down the (from left to right) a, b, and c axes.



Supplementary figure S15. Li_8P_{32} supercell visualised down the (from left to right) a, b, and c axes.



Supplementary figure S16. Li_4P_{32} supercells derived from relaxed Li_8P_{32} to remove half of Li in different configurations. Visualised down the (from top to bottom) free view near a axis, a, b, and c axes.

CRYSTAL17 Input Scripts

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LiP32

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ANDERSON
TOLINTEG
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SCFDIR
SHRINK
4 4
MAXCYCLE
300
FMIXING
90
TOLDEE
7
SPINLOCK
1 30
END
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Li2P32 (Same layer)

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0 0 0
1
6.61313933    10.98605837     8.69146692    85.754139  90.100148  89.653186
34
15    -9.884418480593E-03  1.011129186927E-01  9.079619762206E-03
15    -6.775969577570E-03 -1.098324504204E-01 -3.653841516840E-02
15    -2.425967879221E-04  4.095432763094E-01  2.958291140049E-01
15    -1.834445481705E-03 -3.883980390474E-01  2.016566307318E-01
15     2.411785508452E-01 -3.898994057021E-01  2.518409181104E-02
15     2.487598419485E-01  4.003334285102E-01 -2.538807965154E-02
15     2.421271064661E-01 -1.143320545984E-01  2.738441911035E-01
15     2.440627871413E-01  8.668411948299E-02  1.755505957948E-01
15    -9.033729545102E-03  8.343074834916E-02 -4.863285518827E-01
15    -6.409368582418E-03 -1.138972728213E-01  4.468362129923E-01
15    -5.827442091986E-03  4.132371612367E-01 -1.910428910643E-01
15    -6.626837228151E-03 -3.873424135446E-01 -2.933842724150E-01
15     2.449805285201E-01 -3.878722655267E-01 -4.625090030364E-01
15     2.455630730213E-01  4.135181703472E-01  4.724514784589E-01
15     2.375226306741E-01 -1.153986670224E-01 -2.104274173888E-01
15     2.338811975668E-01  8.569699422472E-02 -3.084159463983E-01
15     4.937218587670E-01  9.159109138786E-02  1.178673204638E-03
15     4.921294338141E-01 -1.121872585149E-01 -4.323519138425E-02
15     4.874202124188E-01  4.288186929561E-01  2.936063451434E-01
15     4.899532972089E-01 -3.730098696433E-01  1.957737912010E-01
15    -2.536346732254E-01 -3.858626948260E-01  3.109091355134E-02
15    -2.539175231334E-01  4.115843714307E-01 -1.896951770494E-02
15    -2.582792529057E-01 -1.050243596007E-01  2.767770111798E-01
15    -2.613143128535E-01  9.743595164406E-02  1.783051869425E-01
15     4.871917664551E-01  7.411463035821E-02 -4.711741570725E-01
15     4.908786260995E-01 -1.183297241331E-01  4.476834145733E-01
15    -4.986693794883E-01  4.063795544467E-01 -1.945904535037E-01
15     4.955703716536E-01 -3.937190036208E-01 -2.911492711477E-01
15    -2.566324978116E-01 -3.884664348675E-01 -4.647281592926E-01
15    -2.586798857637E-01  4.169245031480E-01  4.567112336017E-01
15    -2.531354453930E-01 -1.288233682686E-01 -2.071409986002E-01
15    -2.545367310607E-01  6.723915844295E-02 -3.137931213584E-01
3     -2.306982028797E-01  2.819773583809E-01 -3.186239955352E-01
3      4.718094296900E-01  2.105771528096E-01  3.119739385477E-01
OPTGEOM
ENDOPT
END
15 10
0 0 7 2.0 1.0
```

```
  52426.999233      0.0005520716410
  7863.2660552      0.0042678595308
  1789.5227333      0.0219315291860
  506.27300165      0.0856671683730
  164.60698546      0.2484068660500
  58.391918722      0.4633675397100
  21.643663201      0.3535055815600
0 0 3 2.0 1.0
  99.013837620      0.0218956799580
  30.550439817      0.0956504702950
  5.4537087661     -0.2945427018600
0 0 2 2.0 1.0
  2.6503362563      1.3294381200000
  1.2726688867      0.6610939647300
0 0 1 0.0 1.0
  0.3072409700      1.0000000000000
0 0 1 0.0 1.0
  0.1202708300      1.0000000000000
0 2 5 6.0 1.0
  472.27219248      0.0025710623052
  111.58882756      0.0202502979990
  35.445936418      0.0915807167870
  12.990776875      0.2574945401400
  5.0486221658      0.4286289975800
0 2 1 3.0 1.0
  1.8889755200      1.0000000000000
0 2 1 0.0 1.0
  0.4424064200      1.0000000000000
0 2 1 0.0 1.0
  0.1573225300      1.0000000000000
0 3 1 0.0 1.0
  0.5061295000      1.0000000000000
3 5
0 0 6 2.0 1.0
 6269.2628010 0.00020540968826
 940.31612431 0.00159165540890
 214.22107528 0.00828698297070
 60.759840184 0.03385637424900
 19.915152032 0.11103225876000
 7.3171509797 0.27449383329000
0 0 2 1.0 1.0
 2.9724674216 0.23792456411000
 1.2639852314 0.30765411924000
0 0 1 0.0 1.0
 0.5025516200 1.00000000000000
0 0 1 0.0 1.0
```

```
 0.1000746200 1.00000000000000
0 2 1 0.0 1.0
 0.1450713300 1.00000000000000
99 0
END
DFT
B3LYP-D3
NUMERICAL
XLGRID
END
GCP
METHOD dft/tzvp
END
ANDERSON
TOLINTEG
7 7 7 8 17
SCFDIR
SHRINK
4 4
MAXCYCLE
300
FMIXING
90
TOLDEE
7
END
```

Li2P32 (Different Gallery)

```
CRYSTAL
0 0 0
1
6.63407522    10.74268802    8.74805453    96.544248  90.013366  89.863904
34
15      0.9107140000    0.1002230000    0.1013460000
15      0.9639650000    0.8925230000    0.9856660000
15      0.0851670000    0.3954600000    0.2202050000
15      0.0320410000    0.6068280000    0.1799560000
15      0.2776330000    0.6068200000    0.0080820000
15      0.3308580000    0.3991550000    0.8924120000
15      0.2100640000    0.8910180000    0.3142160000
15      0.1573140000    0.0990270000    0.2753270000
15      0.9046510000    0.0944350000    0.6061040000
15      0.9608280000    0.8908290000    0.4838630000
15      0.0843010000    0.4002690000    0.7184010000
15      0.0315440000    0.6083200000    0.6795140000
15      0.2808110000    0.6084860000    0.5098940000
15      0.3369440000    0.4049000000    0.3876340000
15      0.2095520000    0.8924590000    0.8137960000
15      0.1564070000    0.1039190000    0.7735380000
15      0.4029290000    0.1002070000    0.1014080000
15      0.4554030000    0.8924900000    0.9856210000
15      0.5825350000    0.4064650000    0.2144000000
15      0.5310900000    0.6104640000    0.1747520000
15      0.7861850000    0.6068600000    0.0081220000
15      0.8386890000    0.3991010000    0.8923240000
15      0.7106930000    0.8883530000    0.3138210000
15      0.6597000000    0.0903170000    0.2633820000
15      0.4123900000    0.0950660000    0.6058090000
15      0.4594570000    0.8913590000    0.4841390000
15      0.5818930000    0.4090050000    0.7303680000
15      0.5309580000    0.6109620000    0.6799280000
15      0.7821550000    0.6079930000    0.5096020000
15      0.8292130000    0.4042750000    0.3879520000
15      0.7105260000    0.8888500000    0.8189860000
15      0.6591050000    0.0928500000    0.7793460000
3       0.6207180000    0.2496530000    0.4968870000
3       0.3967050000    0.8283320000    0.6313720000
OPTGEOM
ENDOPT
END
15 10
0 0 7 2.0 1.0
```

```
  52426.999233      0.0005520716410
  7863.2660552      0.0042678595308
  1789.5227333      0.0219315291860
  506.27300165      0.0856671683730
  164.60698546      0.2484068660500
  58.391918722      0.4633675397100
  21.643663201      0.3535055815600
0 0 3 2.0 1.0
  99.013837620      0.0218956799580
  30.550439817      0.0956504702950
  5.4537087661     -0.2945427018600
0 0 2 2.0 1.0
  2.6503362563      1.3294381200000
  1.2726688867      0.6610939647300
0 0 1 0.0 1.0
  0.3072409700      1.0000000000000
0 0 1 0.0 1.0
  0.1202708300      1.0000000000000
0 2 5 6.0 1.0
  472.27219248      0.0025710623052
  111.58882756      0.0202502979990
  35.445936418      0.0915807167870
  12.990776875      0.2574945401400
  5.0486221658      0.4286289975800
0 2 1 3.0 1.0
  1.8889755200      1.0000000000000
0 2 1 0.0 1.0
  0.4424064200      1.0000000000000
0 2 1 0.0 1.0
  0.1573225300      1.0000000000000
0 3 1 0.0 1.0
  0.5061295000      1.0000000000000
3 5
0 0 6 2.0 1.0
 6269.2628010 0.00020540968826
 940.31612431 0.00159165540890
 214.22107528 0.00828698297070
 60.759840184 0.03385637424900
 19.915152032 0.11103225876000
 7.3171509797 0.27449383329000
0 0 2 1.0 1.0
 2.9724674216 0.23792456411000
 1.2639852314 0.30765411924000
0 0 1 0.0 1.0
 0.5025516200 1.00000000000000
0 0 1 0.0 1.0
```

```
 0.1000746200 1.00000000000000
0 2 1 0.0 1.0
 0.1450713300 1.00000000000000
99 0
END
DFT
B3LYP-D3
NUMERICAL
XLGRID
END
GCP
METHOD dft/tzvp
END
ANDERSON
TOLINTEG
7 7 7 8 17
SCFDIR
SHRINK
4 4
MAXCYCLE
300
FMIXING
90
TOLDEE
7
END
```

Li4P32

```
CRYSTAL
0 0 0
1
6.61313933    10.98605837    8.69146692    85.754139  90.100148  89.653186
36
15      0.9062810957    0.0953476965    0.9308727214
15      0.9619925111    0.8903357656    0.9134942864
15      0.0812724286    0.3962114149    0.3863520618
15      0.0292237873    0.6061310753    0.2452544617
15      0.2746964260    0.6078629564    0.0721953943
15      0.3302606724    0.4028927148    0.0546831606
15      0.2074756831    0.8920371036    0.2403957933
15      0.1554972061    0.1019356026    0.0992375600
15      0.9062208745    0.0953867777    0.4308324481
15      0.9620020749    0.8903417432    0.4134541255
15      0.0811450537    0.3961621457    0.8864545189
15      0.0291394995    0.6060723998    0.7452415574
15      0.2746144804    0.6077998624    0.5722067529
15      0.3304132406    0.4028309570    0.5546591876
15      0.2074423498    0.8919803591    0.7404203879
15      0.1553080477    0.1018906724    0.5992921682
15      0.4078825204    0.0949311216    0.9311434855
15      0.4547721965    0.8900980572    0.9129932043
15      0.5769939304    0.4133846333    0.3837932453
15      0.5263816472    0.6144646277    0.2374302714
15      0.7819770196    0.6078719383    0.0727391294
15      0.8287653129    0.4029418757    0.0546704955
15      0.7103421206    0.8836264001    0.2483042913
15      0.6598218684    0.0847028559    0.1018531874
15      0.4077874627    0.0949401245    0.4312413686
15      0.4547210427    0.8900889793    0.4130199532
15      0.5768279210    0.4133971312    0.8837498166
15      0.5263942203    0.6144620759    0.7373404487
15      0.7819417613    0.6079723308    0.5725979372
15      0.8289994019    0.4030596064    0.5545995303
15      0.7103641466    0.8836984187    0.7482876703
15      0.6598059265    0.0847701047    0.6018440608
3       0.6169181680    0.2490829682    0.7427899091
3       0.6169359016    0.2490915034    0.2426484088
3       0.5042667081    0.7465594456    0.2858994165
3       0.7521073196    0.7561124196    0.6094372781
OPTGEOM
ENDOPT
END
```

```
15 10
0 0 7 2.0 1.0
  52426.999233       0.0005520716410
  7863.2660552       0.0042678595308
  1789.5227333       0.0219315291860
  506.27300165       0.0856671683730
  164.60698546       0.2484068660500
  58.391918722       0.4633675397100
  21.643663201       0.3535055815600
0 0 3 2.0 1.0
  99.013837620       0.0218956799580
  30.550439817       0.0956504702950
  5.4537087661      -0.2945427018600
0 0 2 2.0 1.0
  2.6503362563       1.3294381200000
  1.2726688867       0.6610939647300
0 0 1 0.0 1.0
  0.3072409700       1.0000000000000
0 0 1 0.0 1.0
  0.1202708300       1.0000000000000
0 2 5 6.0 1.0
  472.27219248       0.0025710623052
  111.58882756       0.0202502979990
  35.445936418       0.0915807167870
  12.990776875       0.2574945401400
  5.0486221658       0.4286289975800
0 2 1 3.0 1.0
  1.8889755200       1.0000000000000
0 2 1 0.0 1.0
  0.4424064200       1.0000000000000
0 2 1 0.0 1.0
  0.1573225300       1.0000000000000
0 3 1 0.0 1.0
  0.5061295000       1.0000000000000
3 5
0 0 6 2.0 1.0
 6269.2628010 0.00020540968826
 940.31612431 0.00159165540890
 214.22107528 0.00828698297070
 60.759840184 0.03385637424900
 19.915152032 0.11103225876000
 7.3171509797 0.27449383329000
0 0 2 1.0 1.0
 2.9724674216 0.23792456411000
 1.2639852314 0.30765411924000
0 0 1 0.0 1.0
```

```
 0.5025516200 1.00000000000000
0 0 1 0.0 1.0
 0.1000746200 1.00000000000000
0 2 1 0.0 1.0
 0.1450713300 1.00000000000000
99 0
END
DFT
B3LYP-D3
NUMERICAL
XLGRID
END
GCP
METHOD dft/tzvp
END
ANDERSON
TOLINTEG
7 7 7 8 17
SCFDIR
SHRINK
4 4
MAXCYCLE
300
FMIXING
90
TOLDEE
7
END
```

Li8P32

CRYSTAL
0 0 0
1
6.61313933 10.98605837 8.69146692 85.754139 90.100148 89.653186
40
15 0.9062810957 0.0953476965 0.9308727214
15 0.9619925111 0.8903357656 0.9134942864
15 0.0812724286 0.3962114149 0.3863520618
15 0.0292237873 0.6061310753 0.2452544617
15 0.2746964260 0.6078629564 0.0721953943
15 0.3302606724 0.4028927148 0.0546831606
15 0.2074756831 0.8920371036 0.2403957933
15 0.1554972061 0.1019356026 0.0992375600
15 0.9062208745 0.0953867777 0.4308324481
15 0.9620020749 0.8903417432 0.4134541255
15 0.0811450537 0.3961621457 0.8864545189
15 0.0291394995 0.6060723998 0.7452415574
15 0.2746144804 0.6077998624 0.5722067529
15 0.3304132406 0.4028309570 0.5546591876
15 0.2074423498 0.8919803591 0.7404203879
15 0.1553080477 0.1018906724 0.5992921682
15 0.4078825204 0.0949311216 0.9311434855
15 0.4547721965 0.8900980572 0.9129932043
15 0.5769939304 0.4133846333 0.3837932453
15 0.5263816472 0.6144646277 0.2374302714
15 0.7819770196 0.6078719383 0.0727391294
15 0.8287653129 0.4029418757 0.0546704955
15 0.7103421206 0.8836264001 0.2483042913
15 0.6598218684 0.0847028559 0.1018531874
15 0.4077874627 0.0949401245 0.4312413686
15 0.4547210427 0.8900889793 0.4130199532
15 0.5768279210 0.4133971312 0.8837498166
15 0.5263942203 0.6144620759 0.7373404487
15 0.7819417613 0.6079723308 0.5725979372
15 0.8289994019 0.4030596064 0.5545995303
15 0.7103641466 0.8836984187 0.7482876703
15 0.6598059265 0.0847701047 0.6018440608
3 0.6169181680 0.2490829682 0.7427899091
3 0.6169359016 0.2490915034 0.2426484088
3 0.5042667081 0.7465594456 0.2858994165
3 0.7521073196 0.7561124196 0.6094372781
3 0.4112187034 0.7671334354 0.4686589808
3 0.3580253593 0.7604107427 0.8341333649
3 0.0910754882 0.3014827500 0.4554868998

```
3        0.3380851782      0.2829103739      0.6074209063
OPTGEOM
ENDOPT
END
15 10
0 0 7 2.0 1.0
  52426.999233       0.0005520716410
  7863.2660552       0.0042678595308
  1789.5227333       0.0219315291860
  506.27300165       0.0856671683730
  164.60698546       0.2484068660500
  58.391918722       0.4633675397100
  21.643663201       0.3535055815600
0 0 3 2.0 1.0
  99.013837620       0.0218956799580
  30.550439817       0.0956504702950
  5.4537087661      -0.2945427018600
0 0 2 2.0 1.0
  2.6503362563       1.3294381200000
  1.2726688867       0.6610939647300
0 0 1 0.0 1.0
  0.3072409700       1.0000000000000
0 0 1 0.0 1.0
  0.1202708300       1.0000000000000
0 2 5 6.0 1.0
  472.27219248       0.0025710623052
  111.58882756       0.0202502979990
  35.445936418       0.0915807167870
  12.990776875       0.2574945401400
  5.0486221658       0.4286289975800
0 2 1 3.0 1.0
  1.8889755200       1.0000000000000
0 2 1 0.0 1.0
  0.4424064200       1.0000000000000
0 2 1 0.0 1.0
  0.1573225300       1.0000000000000
0 3 1 0.0 1.0
  0.5061295000       1.0000000000000
3 5
0 0 6 2.0 1.0
 6269.2628010 0.00020540968826
 940.31612431 0.00159165540890
 214.22107528 0.00828698297070
 60.759840184 0.03385637424900
 19.915152032 0.11103225876000
 7.3171509797 0.27449383329000
```

0 0 2 1.0 1.0
 2.9724674216 0.23792456411000
 1.2639852314 0.30765411924000
0 0 1 0.0 1.0
 0.5025516200 1.00000000000000
0 0 1 0.0 1.0
 0.1000746200 1.00000000000000
0 2 1 0.0 1.0
 0.1450713300 1.00000000000000
99 0
END
DFT
B3LYP-D3
NUMERICAL
XLGRID
END
GCP
METHOD dft/tzvp
END
ANDERSON
TOLINTEG
7 7 7 8 17
SCFDIR
SHRINK
4 4
MAXCYCLE
300
FMIXING
90
TOLDEE
7
END