Supplementary Information

Synthesis and characterization of highly porous borazine-linked polymers and their performance in hydrogen storage application

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Section S1: *Synthetic Procedures*

General Synthetic Procedures.

All starting materials, unless noted otherwise, were obtained from Thermo Fisher Scientific Inc. and used without further purification. Dichloromethane was distilled from calcium hydride, and toluene was distilled from sodium. All products were handled under a nitrogen atmosphere using glovebox or Schlenk line techniques. Elemental analyses were performed by Midwest Microlab, Indianapolis, IN. Higher carbon and hydrogen contents may result from residual hydrocarbons in the cavities.

p-Phenylenediamine was purchased from Acros Chemicals and was purified by sublimation prior to use, and 1,3,5-tris-(4-aminophenyl)benzene was prepared according to literature methods.[1]

Synthesis of BLP-1(Br). *p*-Phenylenediamine (0.30 g, 2.77 mmol) was dissolved in 60 mL of dry dichloromethane under a nitrogen atmosphere and cooled to -78 ºC. While stirring, 6.5 mL of 1M boron tribromide (6.5 mmol) in dichloromethane was added. After 30 minutes of stirring, all of the dichloromethane was removed under reduced pressure and replaced with 60 mL of dry toluene. The mixture was refluxed overnight and taken into a glovebox. The white solid was filtered over a medium glass frit and rinsed with dry dichloromethane. The product was soaked in dry dichloromethane for 24 hours at which point the solvent was decanted, and fresh, dry dichloromethane was replenished. Decantation and addition of fresh solvent was repeated once more. The solid was then activated at 80 ºC under reduced pressure for 18 hours to afford **BLP-1(Br)** (0.62 g, 78%) as a white solid. Anal. Calcd. for $C_{18}H_{12}B_6N_6Br_6$: C, 25.24; H, 1.41; N, 9.81. Found: C, 27.65; H, 2.26; N, 9.97.

Synthesis of BLP-1(Cl). In a similar fashion to BLP-1(Br), 0.30 g (2.77 mmol) of *p*-phenylenediamine was dissolved in 60 mL of dry dichloromethane under a nitrogen atmosphere and cooled to -78 ºC. While stirring, 6.5 mL of 1M boron trichloride (6.5 mmol) in dichloromethane was added. After 30 minutes of stirring, all of the dichloromethane was removed under reduced pressure and replaced with 60 mL of dry toluene. The mixture was refluxed overnight and taken into a glovebox. The white solid was filtered over a medium glass frit and rinsed with dry dichloromethane. The product was soaked in dry dichloromethane for 24 hours at which point the solvent was decanted, and fresh, dry dichloromethane was replenished. Decantation and addition of fresh solvent was repeated once more. The solid was then activated at 80 ºC under reduced pressure for 18 hours to afford **BLP-1(Cl)** (0.51 g, 94%) as a white solid. Anal. Calcd. for $C_{18}H_{12}B_6N_6Cl_6$: C, 36.65; H, 2.05; N, 14.25. Found: C, 37.77; H, 2.87; N, 13.12.

Synthesis of BLP-2(Br). In a similar fashion to BLP-1(Br), 0.30 g (0.85 mmol) of 1,3,5-tris-(4-aminophenyl)benzene was dissolved in 60 mL of dry dichloromethane under a nitrogen atmosphere and cooled to -78ºC. While stirring, 4.0 mL of 1M boron tribromide (4.0 mmol) in dichloromethane was added. After 30 minutes of stirring, all of the dichloromethane was removed under reduced pressure and replaced with 60 mL of dry toluene. The mixture was refluxed overnight and taken into a glovebox. The off-white solid was filtered over a medium glass frit and rinsed with dry dichloromethane. The product was soaked in dry dichloromethane for 24 hours at which point the solvent was decanted, and fresh, dry dichloromethane was replenished. Decantation and addition of fresh solvent was repeated once more. The solid was then activated at 80 ºC under reduced pressure for 18 hours to afford **BLP-2(Br)** (0.32 g, 71%) as an off-white solid. Anal. Calcd. for $C_{24}H_{15}B_3N_3Br_3$: C, 46.68; H, 2.45; N, 6.81. Found: C, 48.83; H, 2.95; N, 6.89.

Synthesis of BLP-2(Cl). In a similar fashion to BLP-2(Br), 0.30 g (0.85 mmol) of 1,3,5-tris-(4-aminophenyl)benzene was dissolved in 60 mL of dry dichloromethane under a nitrogen atmosphere and cooled to -78ºC. While stirring, 4.0 mL of 1M boron trichloride (4.0 mmol) in dichloromethane was added. After 30 minutes of stirring, all of the dichloromethane was removed under reduced pressure and replaced with 60 mL of dry toluene. The mixture was refluxed overnight and taken into a glovebox. The off-white solid was filtered over a medium glass frit and rinsed with dry dichloromethane. The product was soaked in dry dichloromethane for 24 hours at which point the solvent was decanted, and fresh, dry dichloromethane was replenished. Decantation and addition of fresh solvent was repeated once more. The solid was then activated at 80 ºC under reduced pressure for 18 hours to afford **BLP-2(Cl)** (0.30 g, 80%) as an off-white solid. Anal. Calcd. for $C_{24}H_{15}B_3N_3Cl_3$: C, 59.53; H, 3.12; N, 8.68. Found: C, 58.90; H, 3.66; N, 8.49.

Section S2: *FT-IR Spectroscopy for BLPs and the Starting Materials*

FT-IR spectra were obtained as KBr pellets using a Nicolet Nexus 670 FT-IR spectrometer. FT-IR spectra were obtained to verify the production of the intended products coupled with the loss of starting material. The fading of certain peaks like amine stretching combined with the appearance of borazine-characteristic peaks supports the production of the intended products.

Figure S1: IR spectra of an activated BLP-1(Br) sample with its starting material, p-phenylenediamine. The largely diminished amine stretching and bending bands indicate the consumption of the starting material, p-phenylenediamine. The peaks around 1400 and 1000 cm^{-1} indicate the closing of the boron-nitrogen adduct into the ring system borazine[2].

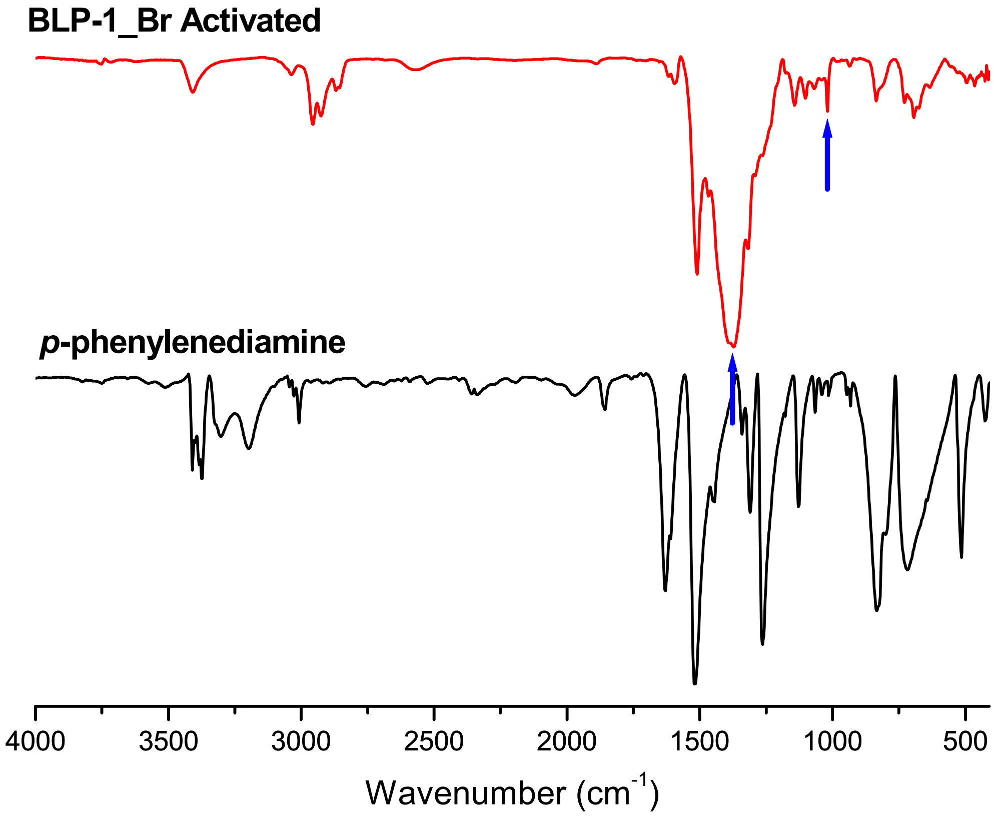


Figure S2: IR spectra of an activated BLP-1(Cl) sample with its starting material, p-phenylenediamine. The largely diminished amine stretching and bending bands indicate the consumption of the starting material, p-phenylenediamine. The peaks around 1400 and 1000 cm^{-1} indicate the closing of the boron-nitrogen adduct into the ring system borazine[2].

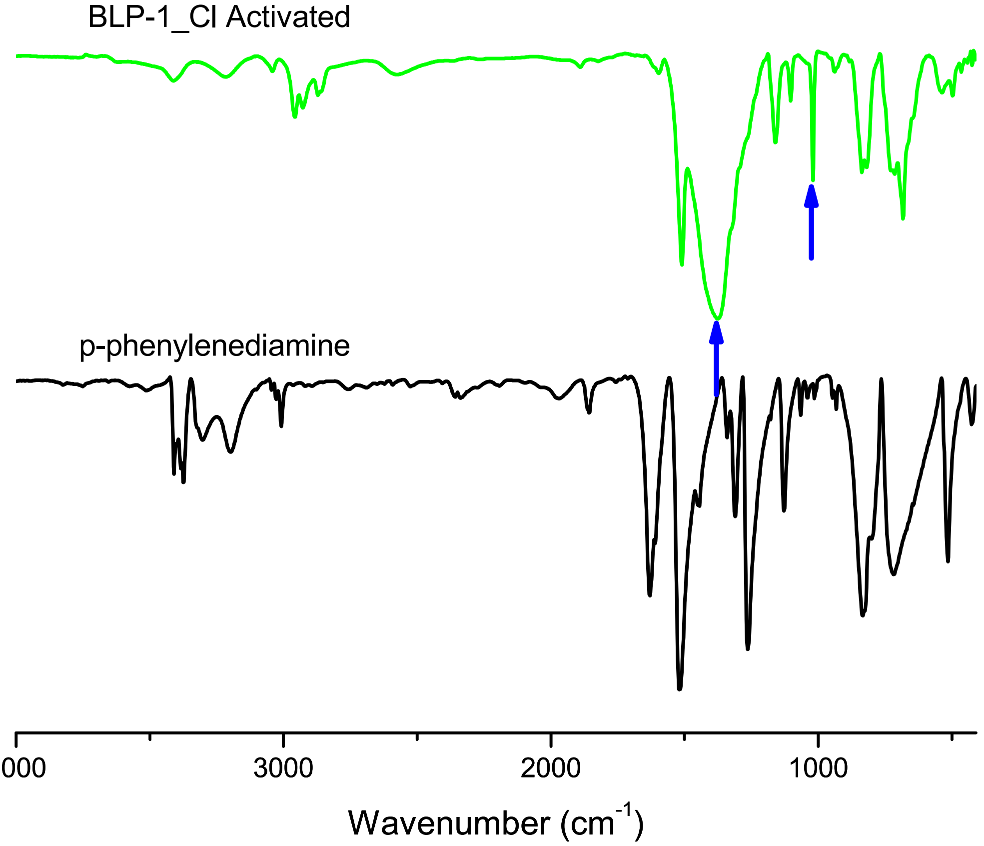


Figure S3: IR spectra of an activated BLP-2(Br) sample with its starting material, p-phenylenediamine. The largely diminished amine stretching and bending bands indicate the consumption of the starting material, p-phenylenediamine. The peaks around 1400 and 1000 cm^{-1} indicate the closing of the boron-nitrogen adduct into the ring system borazine^{2}.

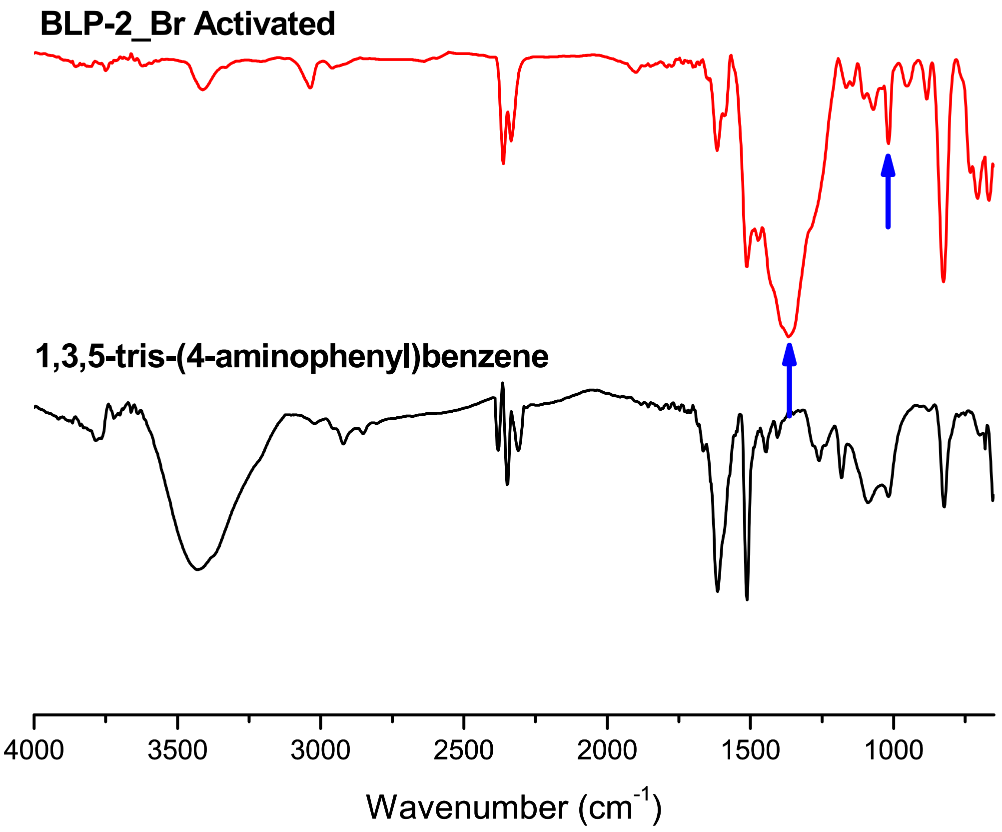
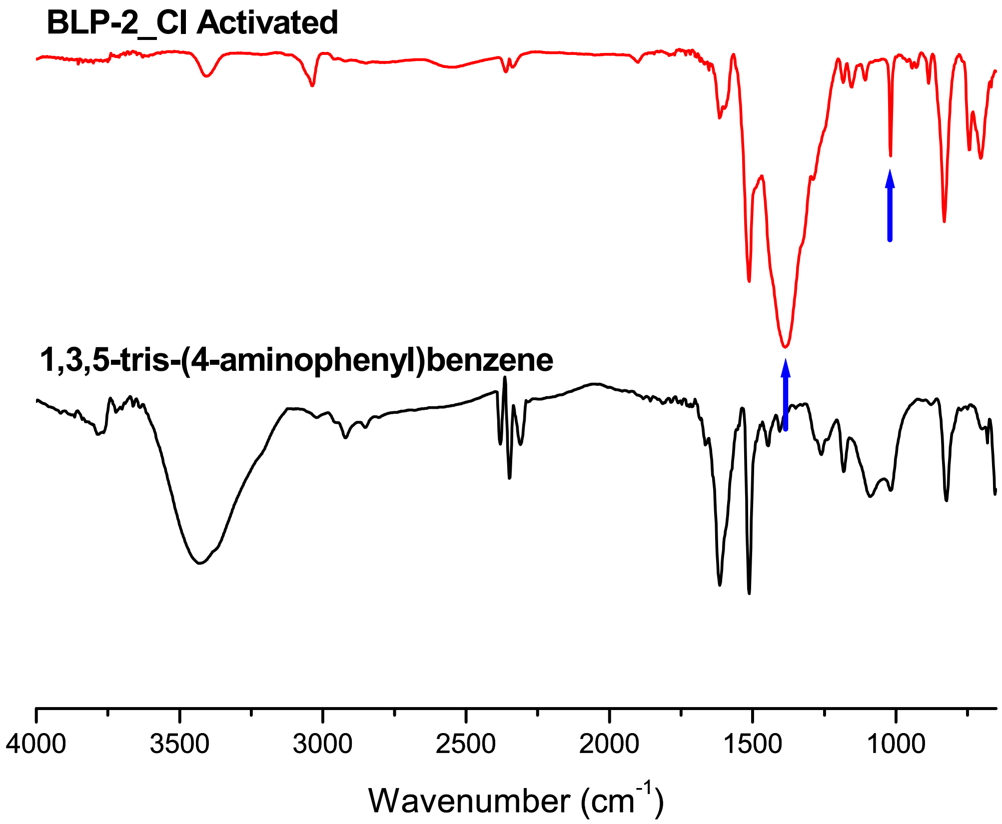


Figure S4: IR spectra of an activated BLP-2(Cl) sample with its starting material, p-phenylenediamine. The largely diminished amine stretching and bending bands indicate the consumption of the starting material, p-phenylenediamine. The peaks around 1400 and 1000 cm^{-1} indicate the closing of the boron-nitrogen adduct into the ring system borazine[2].



Section S3: *Solid-State ^{11}B and ^{13}C Multiple Quantum Magic Angle Spinning (MQMAS) Nuclear Magnetic Resonance*

Solid-state nuclear magnetic resonance (NMR) spectra were recorded at ambient temperature on a Bruker DSX-300 spectrometer using a Bruker magic angle spinning (MAS) probe with 4 mm (O.D.) 80 µL volume zirconia rotors with Kel-F drive caps. All polymers were packed in a nitrogen environment. Cross-polarization with MAS (CPMAS) was used to acquire ^{13}C data at 75.47 MHz. The ^{1}H and ^{13}C ninety-degree pulse widths were both 4 µs, and the CP contact time was 1.5 ms. High power two-pulse phase modulation (TPPM) ^{1}H decoupling was applied during data acquisition. The decoupling frequency corresponded to 72 kHz. The MAS sample spinning rate was 10 kHz. Recycle delays between scans varied between 10 and 30 s, depending upon the sompound as determined by observing no apparent loss in ^{13}C signal intensity from one scan to the next. The ^{13}C chemical shifts are given relative to tetramethylsilane as zero ppm, calibrated using the methane carbon signal of adamantine assigned to 29.46 ppm as a secondary reference.

Multiple quantum MAS (MQMAS) spectroscopy was used to acquire ^{11}B data at 96.29 MHz. The ^{11}B solution-state ninety-degree pulse width was 2 µs. TPPM ^{1}H decoupling was applied during data acquisition. The decoupling frequency corresponded to 72 kHz. The MAS spinning rate was 14.9 kHz. A recycle delay of 3 s was used. The ^{11}B chemical shifts are given relative to BF_3 etherate as zero ppm, calibrated using aqueous boric acid at pH = 4.4 assigned to -19.6 ppm as a secondary reference.

Figure S5: Solid-State ^{11}B NMR Spectrum of BLP-1(Cl).

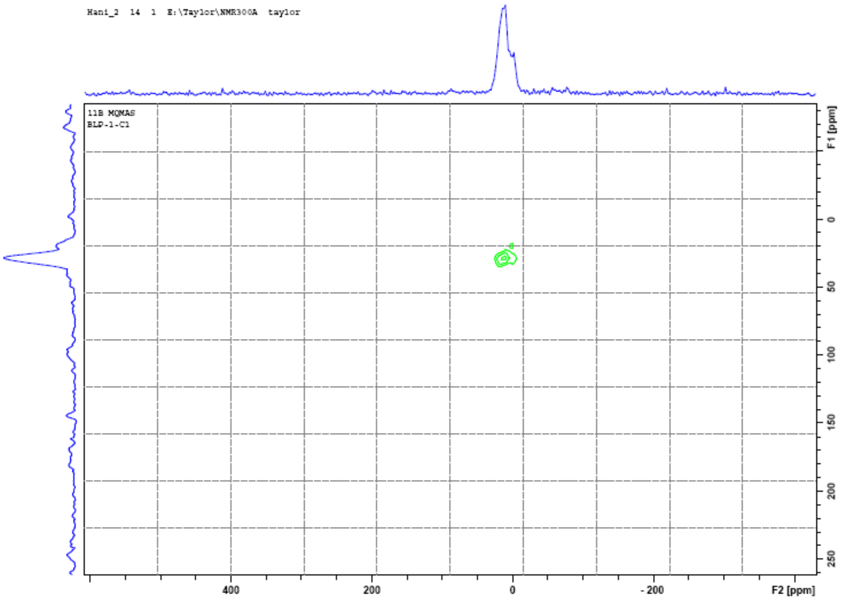


Figure S6: Solid-State ^{11}B NMR Spectrum of BLP-1(Cl).

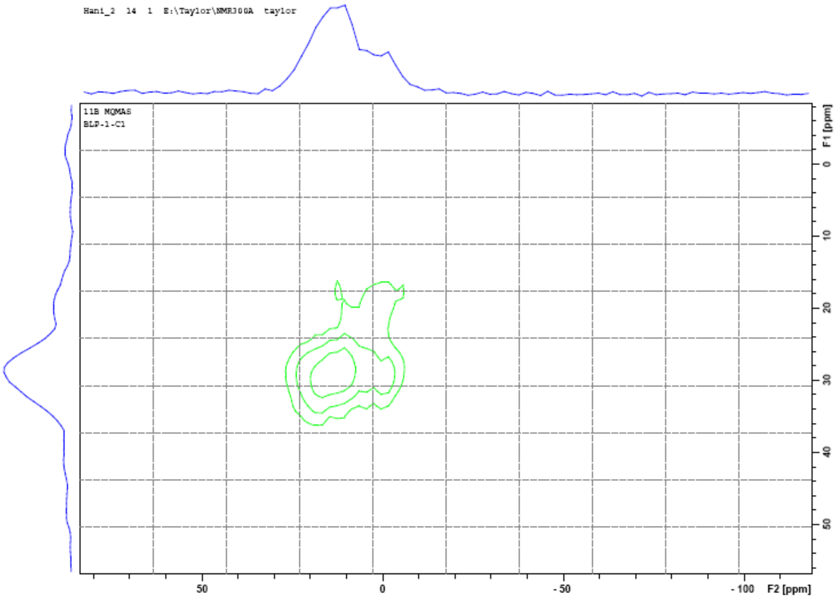
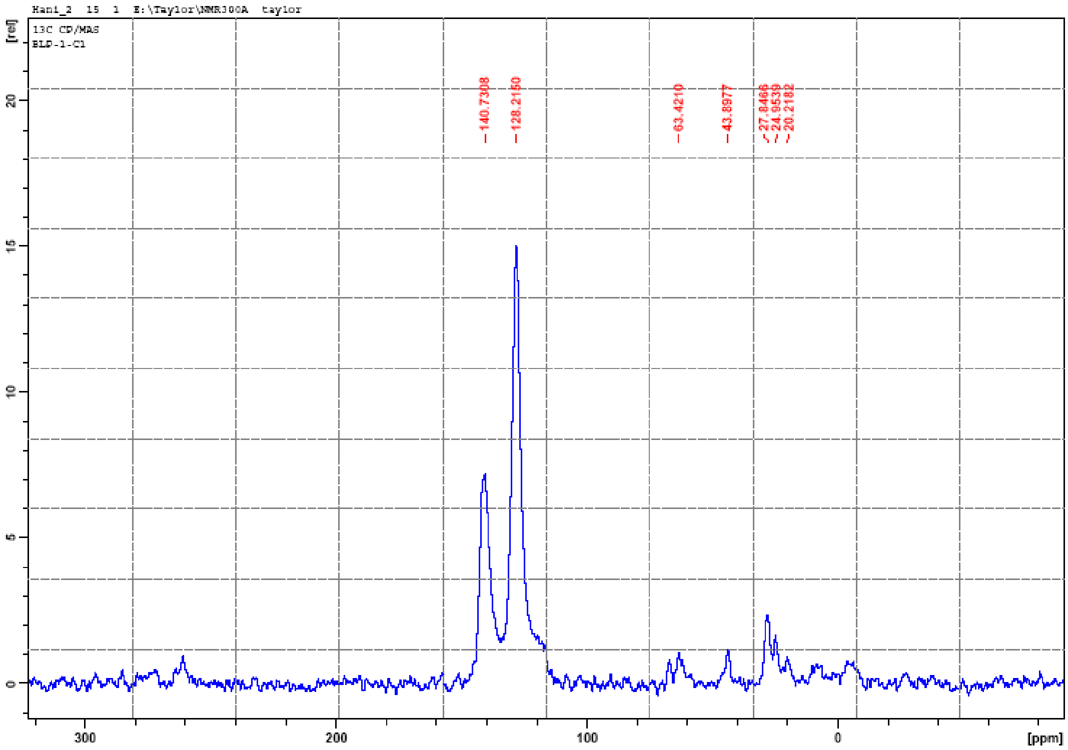
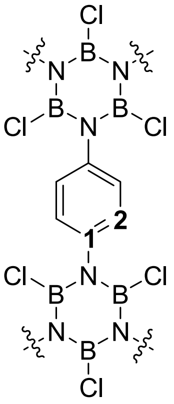


Figure S7: Solid-State ^{13}C NMR Spectrum of BLP-1(Cl). Both of the expected peaks from the starting material are present in BLP-1(Cl). These peaks indicate that the backbone of the arylamine building block survived the reaction.



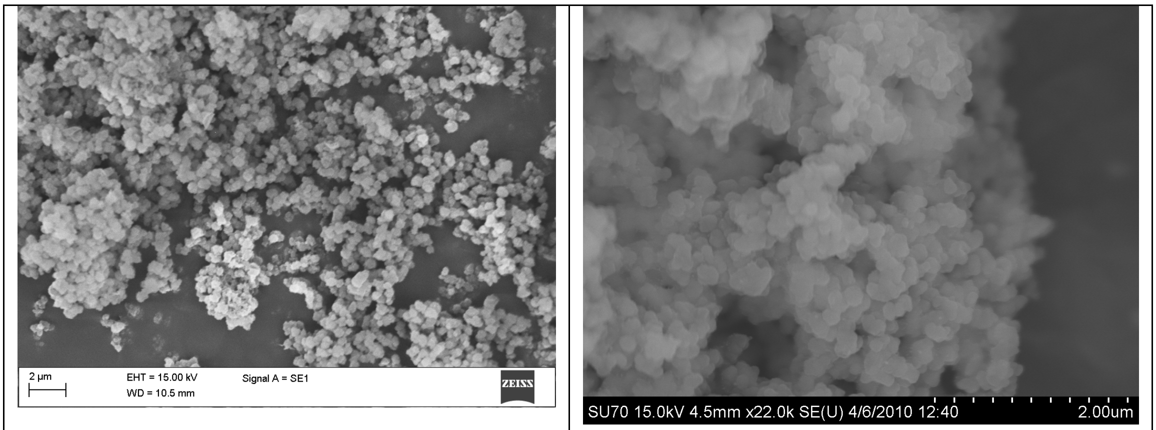


Carbon	Chemical Shift (ppm)
1	140.73
2	128.21

Section S4: *Scanning Electron Microscopy (SEM) Imaging*

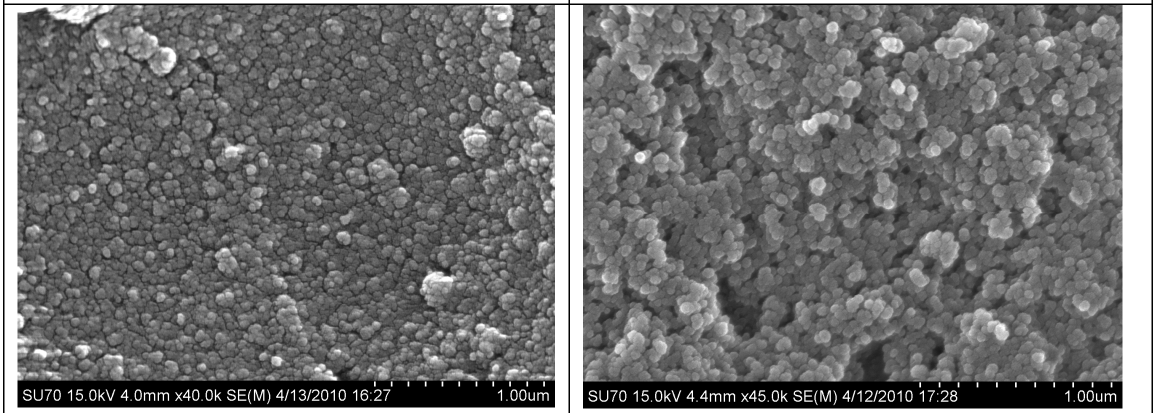
Samples of all polymers were prepared by dispersing the material onto a sticky carbon surface attached to a flat aluminum sample holder. The samples were then gold coated using an EMS (Electron Microscopy Sciences) 550x Sputter Coater at 1x10^{-1} mbar of pressure in a nitrogen atmosphere for 120 seconds while maintaining 20 mA of current. Samples were analyzed on a Zeiss EVO XVP Scanning Electron Microscope using the SEI detector with accelerating voltages ranging from 10 kV to 20 kV.

Figure S8: SEM image of BLPs.



BLP-1(Cl)

BLP-1(Br)



BLP-2(Cl)

BLP-2(Br)

Section S5: *Thermogravimetric Analysis (TGA)*

Thermogravimetric analysis was obtained using a TA Instruments TGA Q5000 analyzer with 50 µL platinum pans to assess the thermal stability of each borazine-linked polymer. Experiments were run at a ramp rate of 5 K/minute under a nitrogen atmosphere.

Figure S9: TGA for an unactivated sample of BLP-1(Br).

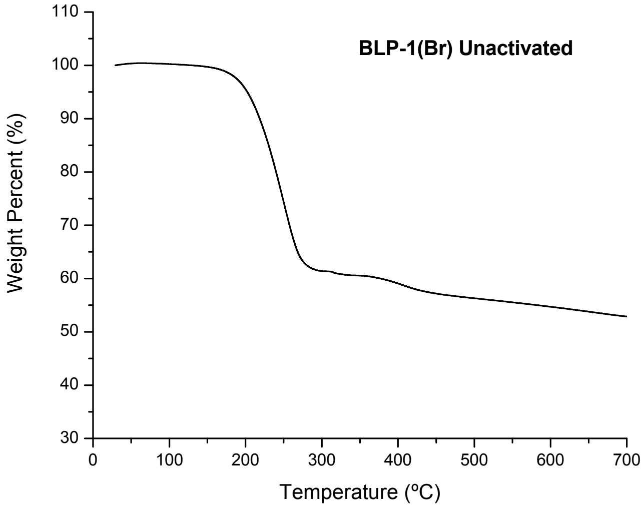


Figure S10: TGA for an unactivated sample of BLP-1(Cl).

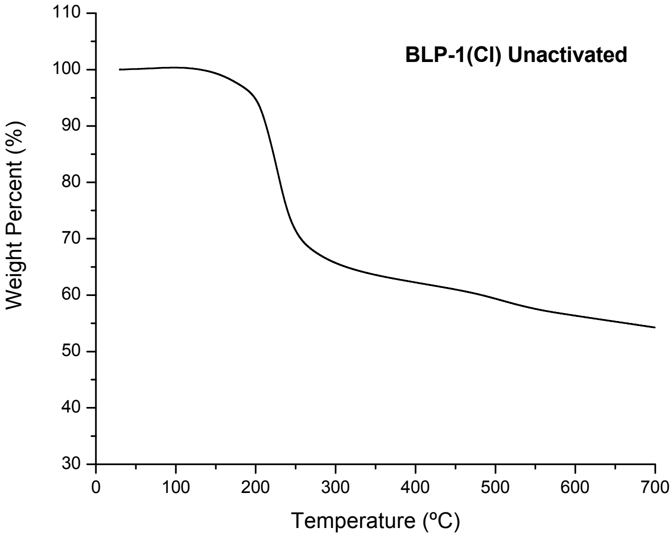


Figure S11: TGA for an unactivated sample of BLP-2(Br).

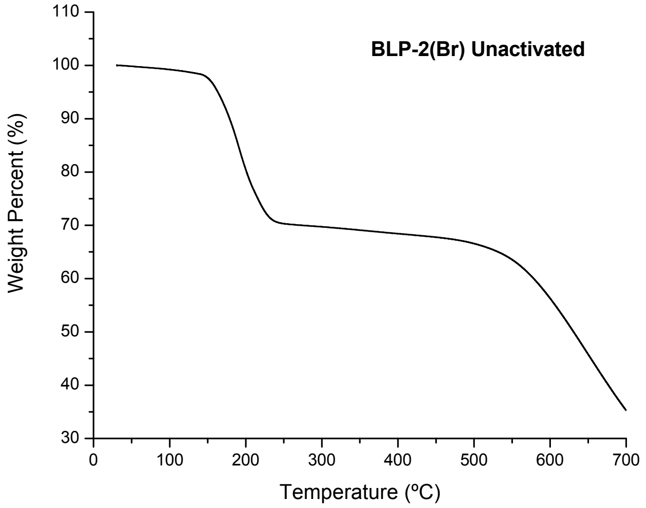
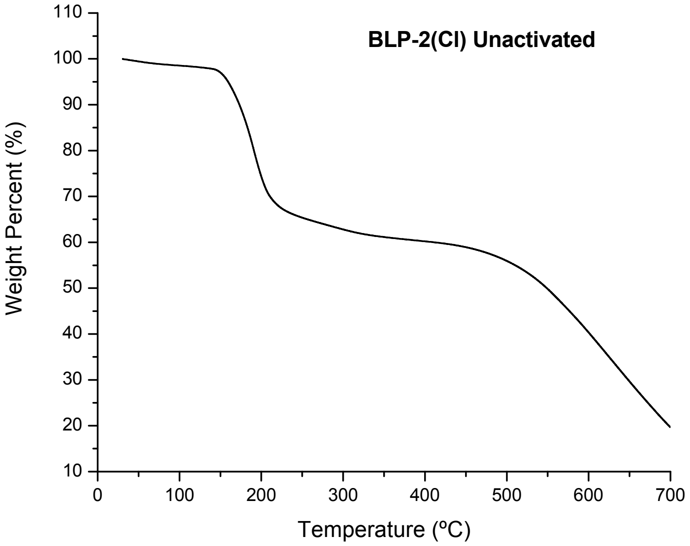


Figure S12: TGA for an unactivated sample of BLP-2(Cl).



Section S6: *Low Pressure (0 – 1.0 bar) Nitrogen and Hydrogen Gas Adsorption Measurements and Hydrogen Isosteric Heat of Adsorption*

Nitrogen experiments were run using a Quantachrome Autosorb 1-C analyzer at 77 K. Pore Size Distributions (PSDs) were calculated using Non-Local Density Functional Theory (NLDFT) on the adsorption branch with a cylindrical pore model on the nitrogen experiments combined with data taken from carbon dioxide sorption experiments performed at 273 K as has been reported previously.[3] Hydrogen sorption experiments were run on the same Quantachrome Autosorb 1-C analyzer at both 77 K and 87 K.

Using the data taken at 77 K and 87 K, the hydrogen isosteric heat of adsorption for each polymer was calculated according to previous reports[4] by solving the virial-type expression:

$$\ln P = \ln N + (1/T)\sum_{i=0}^{m} a_i N^i + \sum_{i=0}^{n} b_i N^i$$

where P is pressure in torr, T is temperature in Kelvin, and N is the mmol of H_2 adsorbed per gram of sample. The values for m and n were varied such that $m \geq n$ and resulted in the best fit as determined by the sum of the squares of the errors. The values for a_0, $a_1, \ldots a_m$ were used in the calculation for the isosteric heat of adsorption, Q_{st}:

$$Q_{st} = -R\sum_{i=0}^{m} a_i N^i$$

The calculated values were plotted as they relate to surface coverage, and the isosteric heat of adsorption values at the point of zero-coverage were highlighted in the text.

Figure S13: Nitrogen isotherm for BLP-1(Br), BLP-1(Cl), BLP-2(Br), and BLP-2(Cl) measured at 77K.

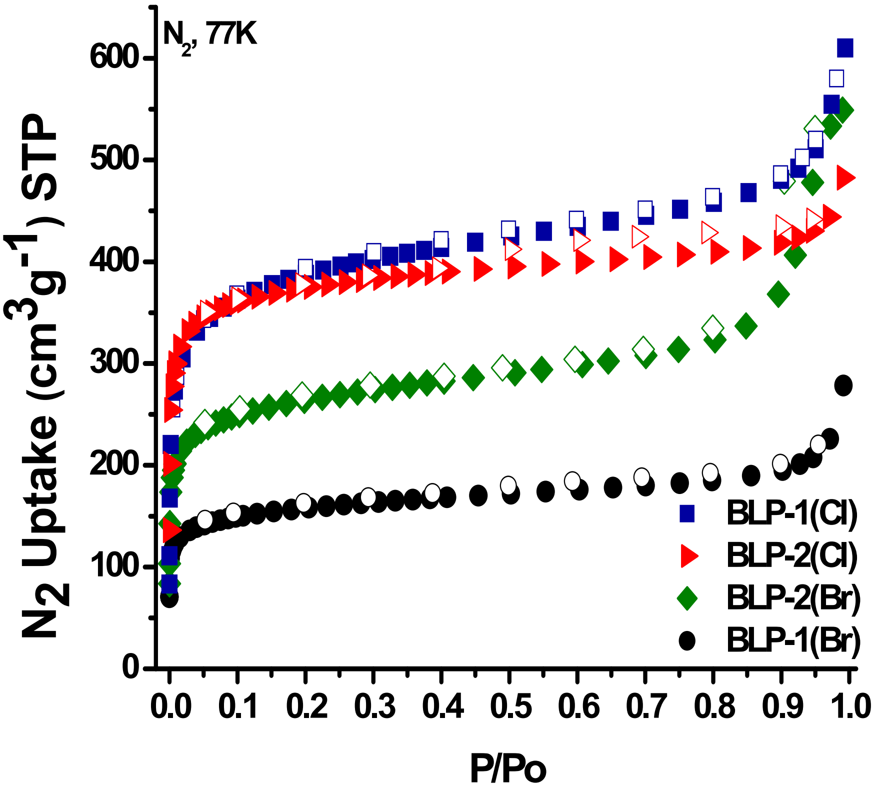


Figure S14: Pore Size Distribution (PSD) for BLP-1(Br) using the NLDFT model.

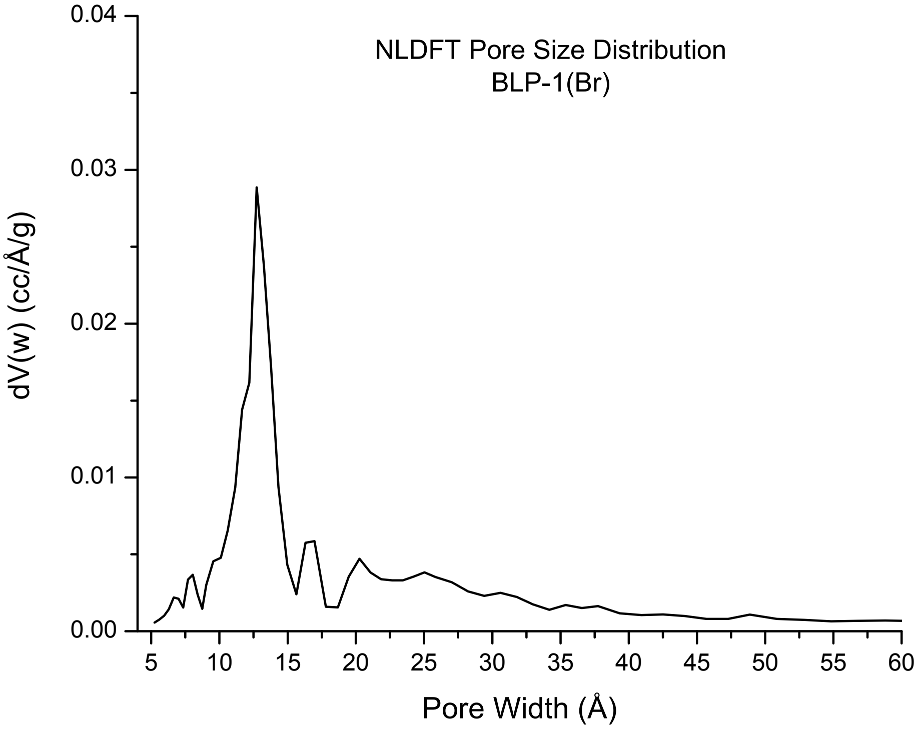


Figure S15: NLDFT calculated isotherm for BLP-1(Br) overlaid with the experimental nitrogen isotherm. A fitting error less than 1% indicates validity of the model.

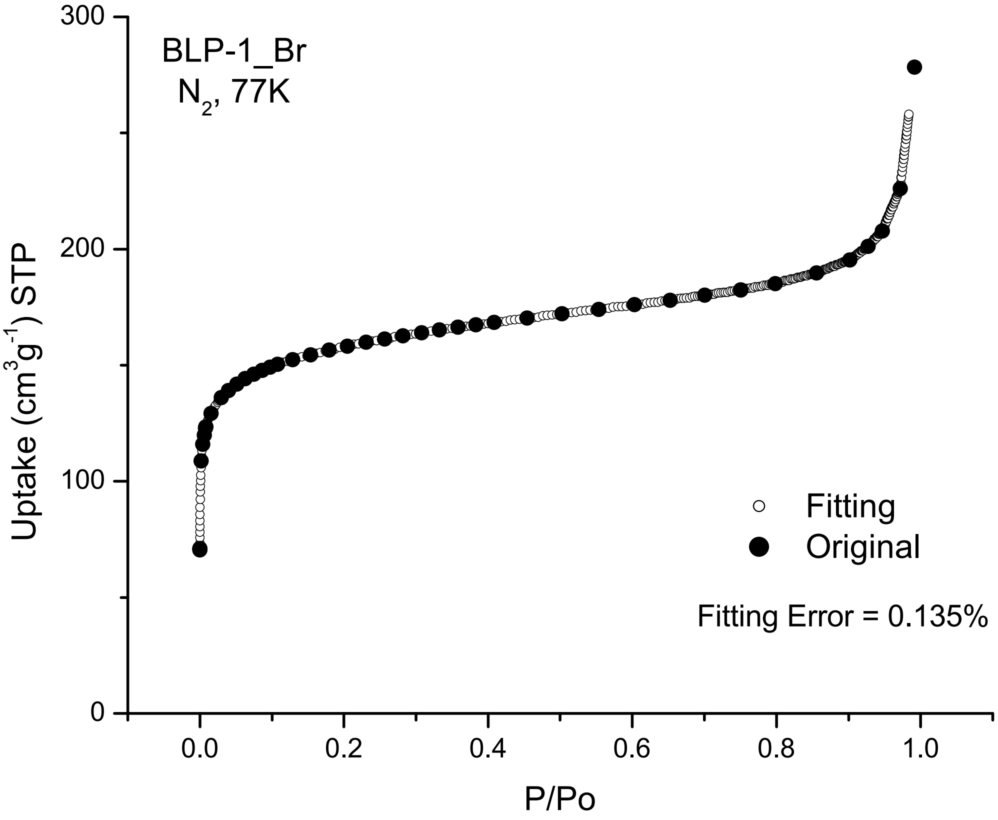


Figure S16: Langmuir plot for BLP-1(Br) calculated from the nitrogen adsorption in the range 0.06-0.30 P/P$_o$.

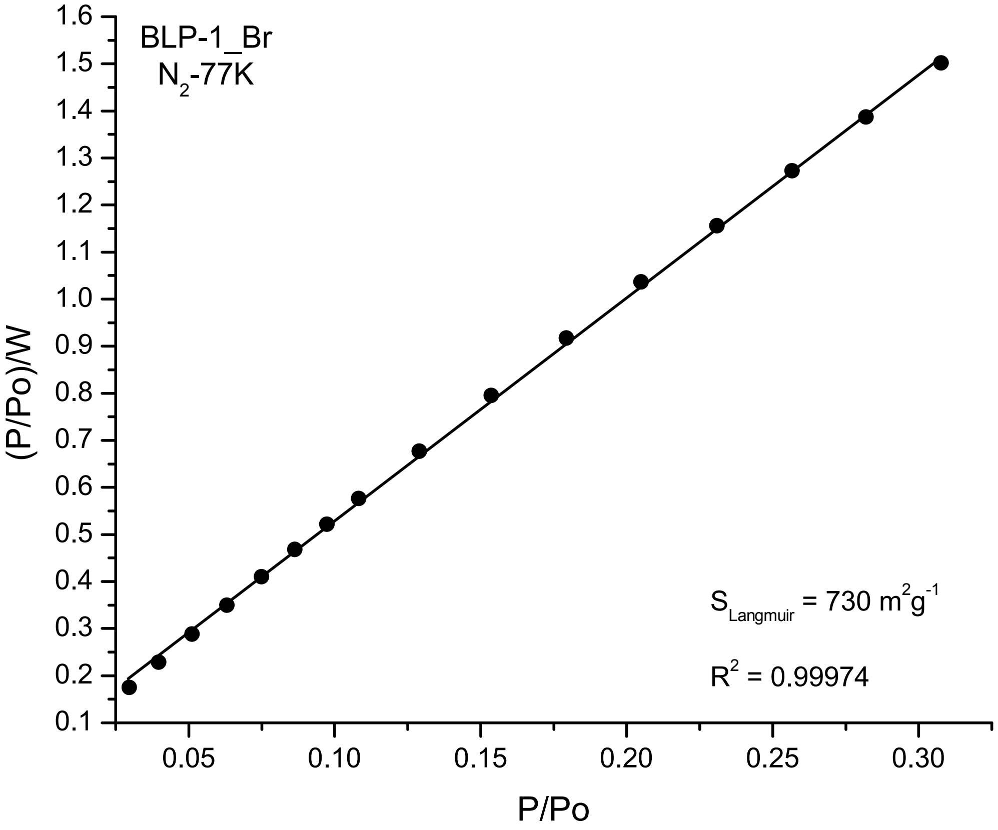


Figure S17: Multipoint BET plot for BLP-1(Br) calculated from the nitrogen adsorption in the range 0.02-0.20 P/P$_o$.

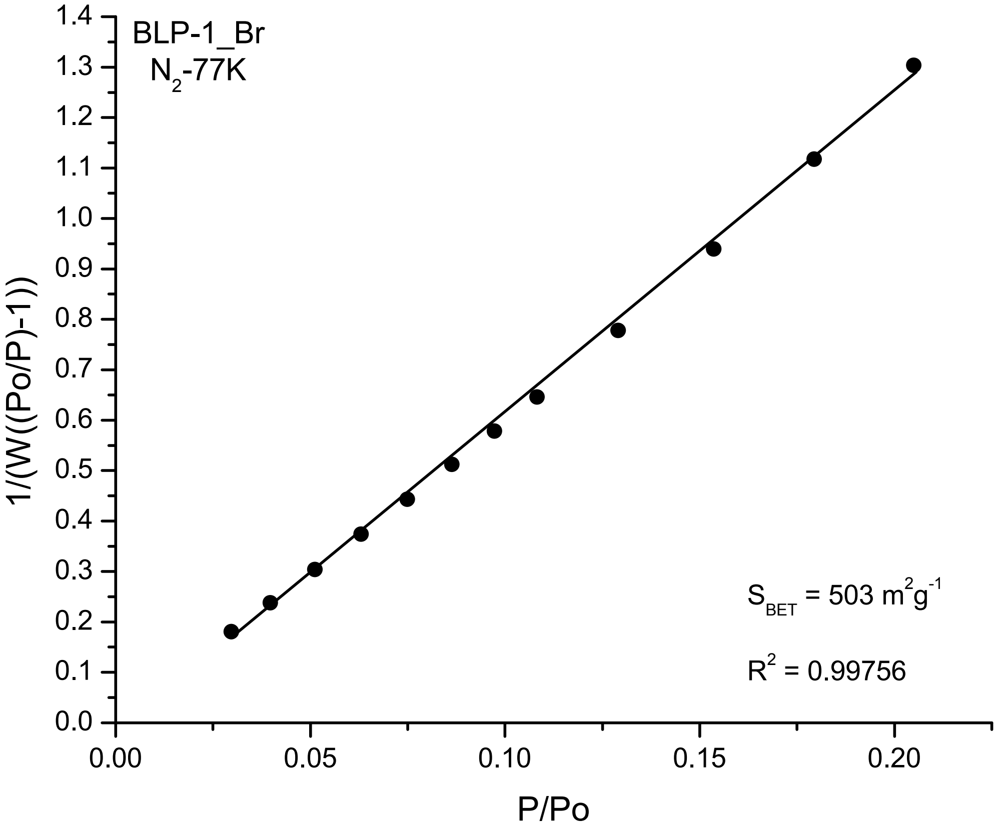


Figure S18: Pore Size Distribution (PSD) for BLP-1(Cl) using the NLDFT model.

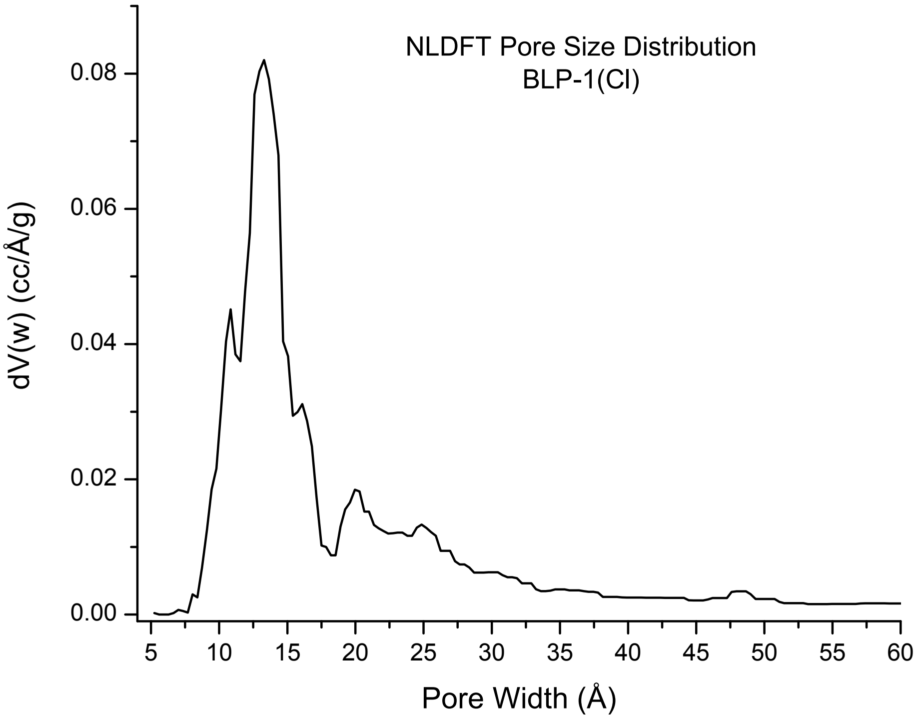


Figure S19: NLDFT calculated isotherm for BLP-1(Cl) overlaid with the experimental nitrogen isotherm. A fitting error less than 1% indicates validity of the model.

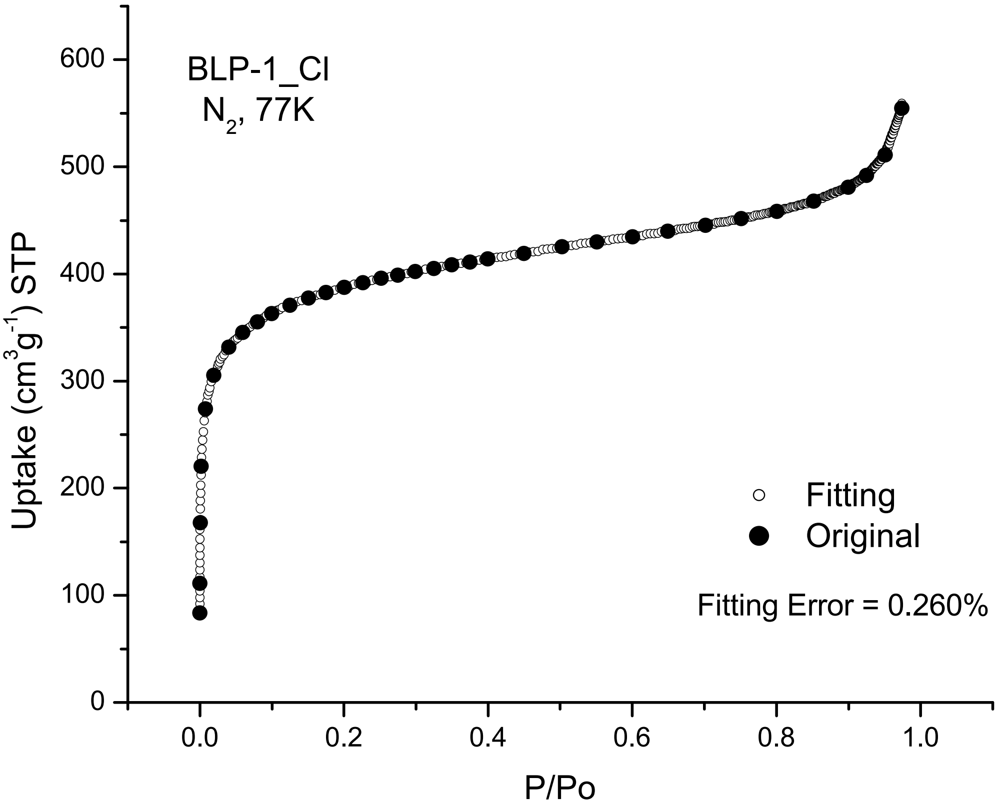


Figure S20: Langmuir plot for BLP-1(Cl) calculated from the nitrogen adsorption in the range 0.06-0.30 P/P_o.

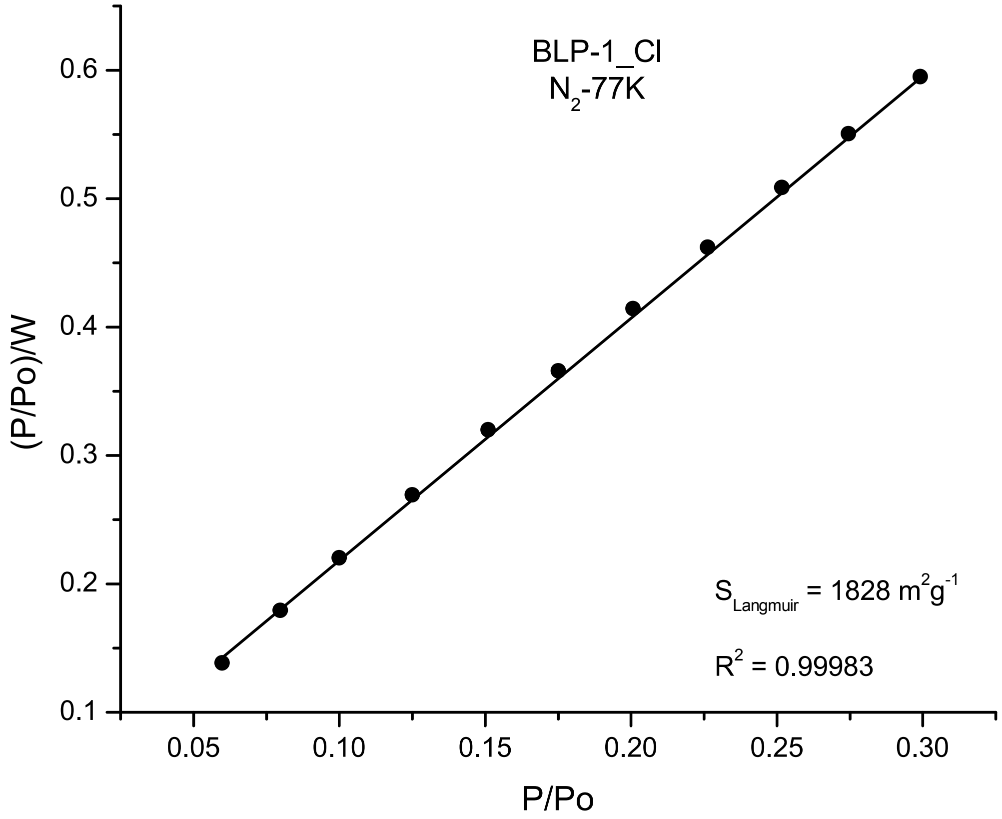


Figure S21: Multipoint BET plot for BLP-1(Cl) calculated from the nitrogen adsorption in the range 0.02-0.20 P/P$_o$.

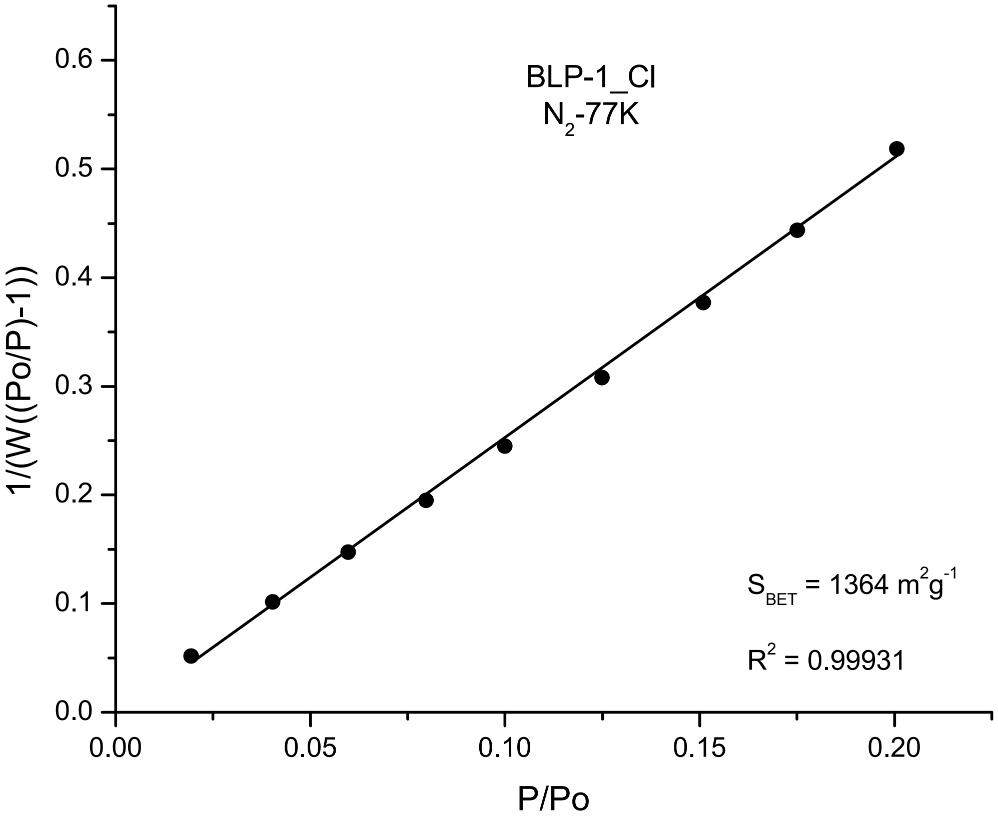


Figure S22: Pore Size Distribution (PSD) for BLP-2(Br) using the NLDFT model.

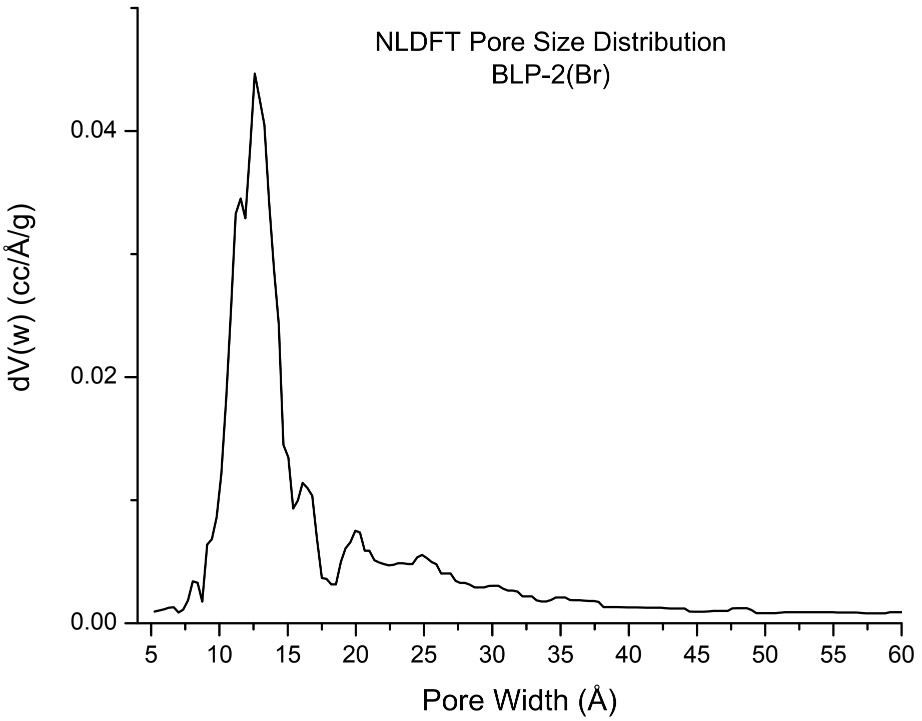


Figure S23: NLDFT calculated isotherm for BLP-2(Br) overlaid with the experimental nitrogen isotherm. A fitting error less than 1% indicates validity of the model.

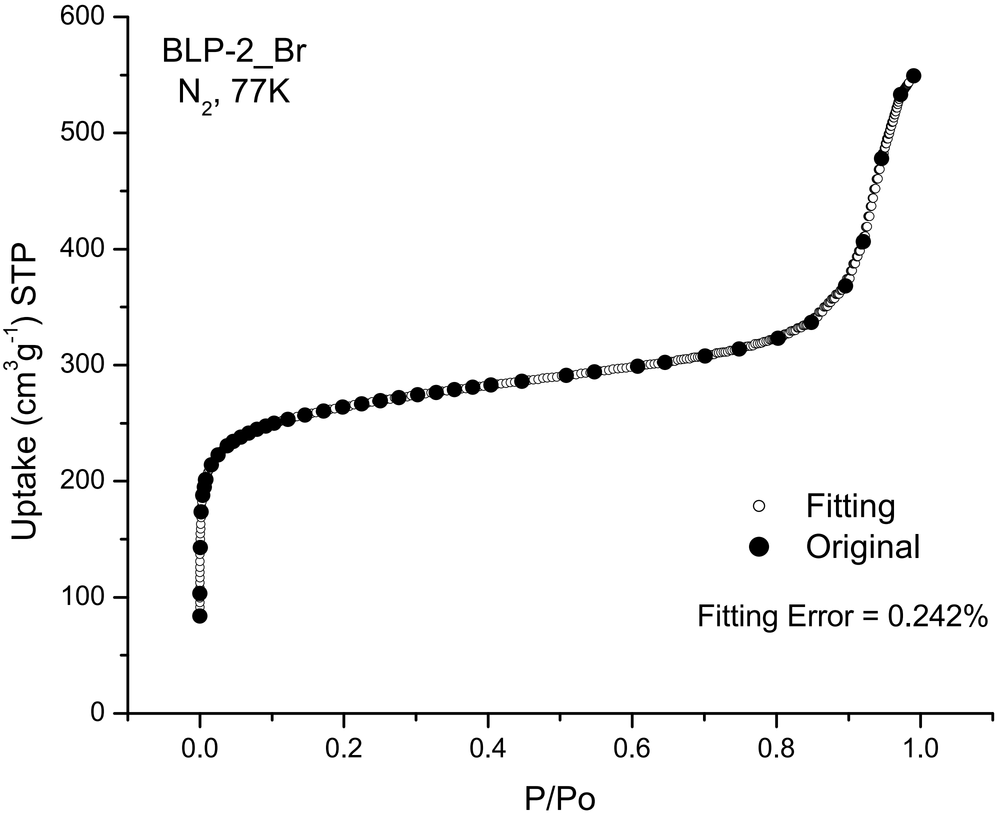


Figure S24: Langmuir plot for BLP-2(Br) calculated from the nitrogen adsorption in the range 0.06-0.30 P/P_o.

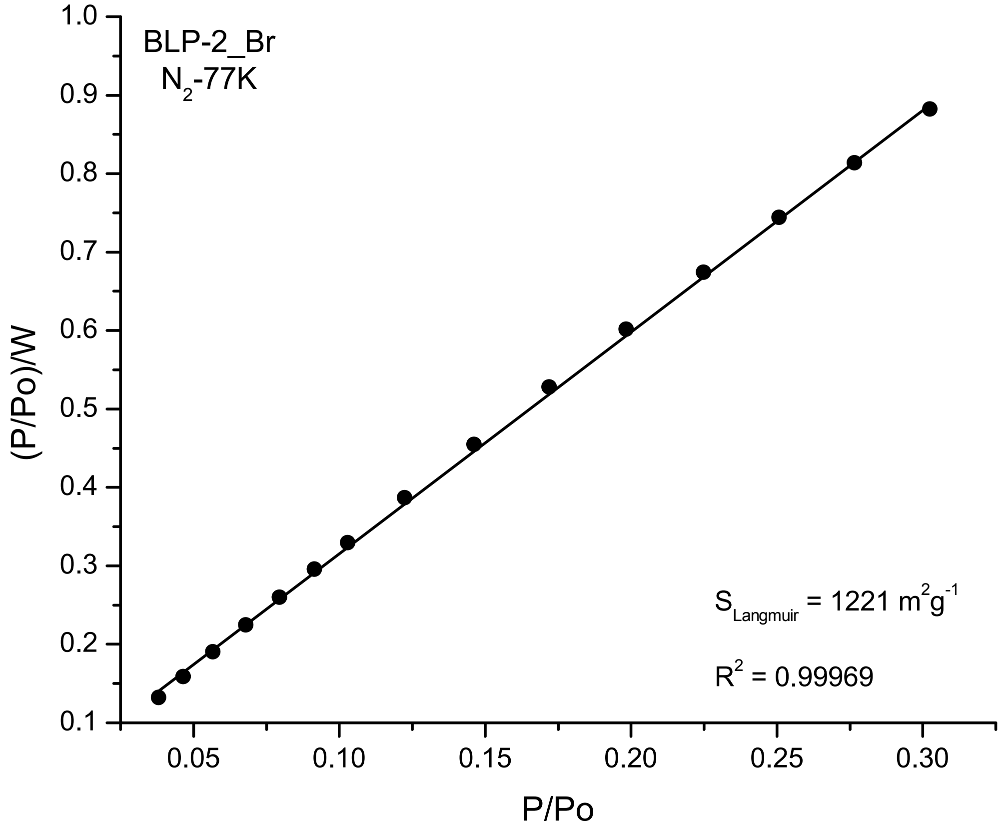


Figure S25: Multipoint BET plot for BLP-2(Br) calculated from the nitrogen adsorption in the range 0.02-0.20 P/P$_o$.

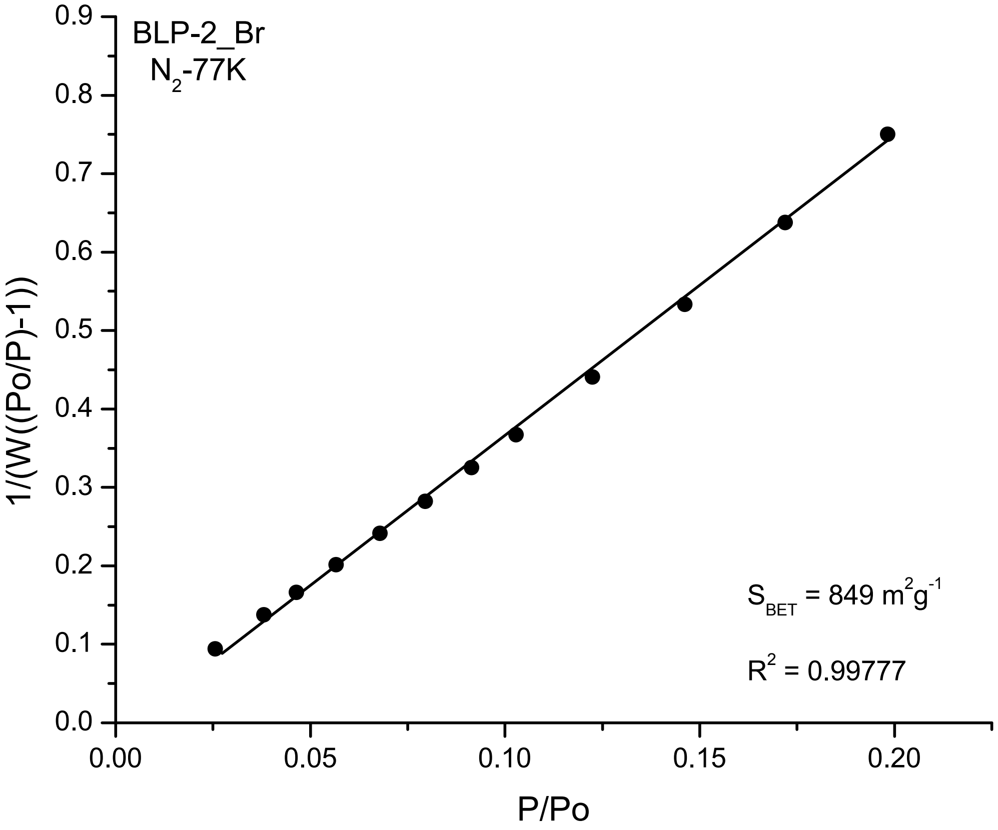


Figure S26: Pore Size Distribution (PSD) for BLP-2(Cl) using the NLDFT model.

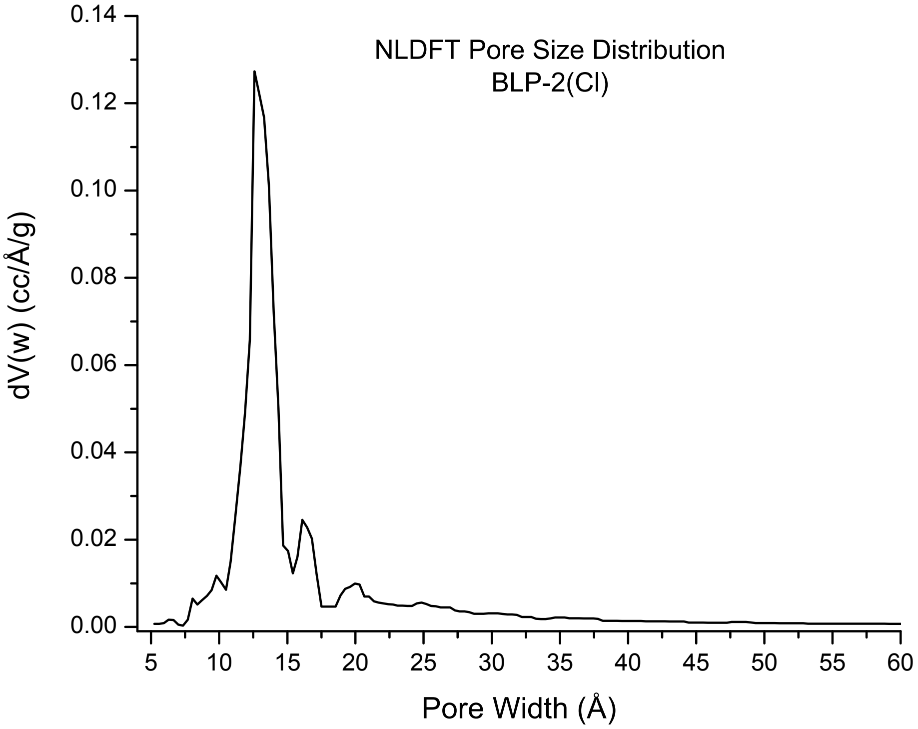


Figure S27: NLDFT calculated isotherm for BLP-2(Cl) overlaid with the experimental nitrogen isotherm. A fitting error less than 1% indicates validity of the model.

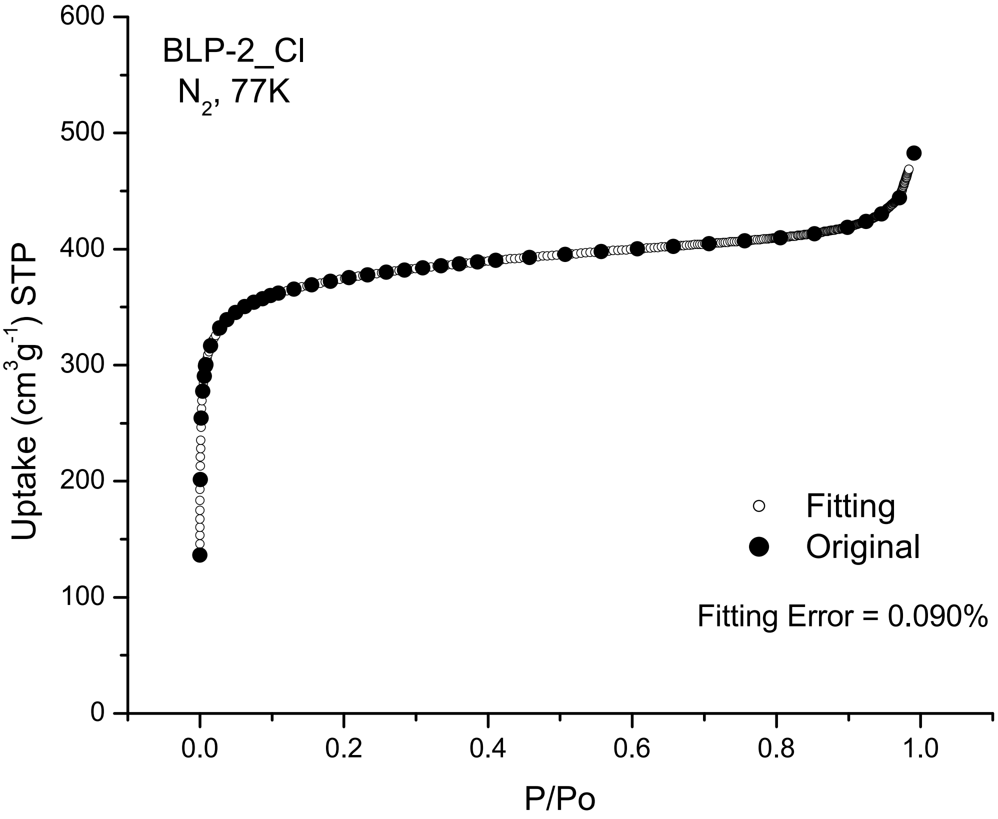


Figure S28: Langmuir plot for BLP-2(Cl) calculated from the nitrogen adsorption in the range 0.06-0.30 P/P$_o$.

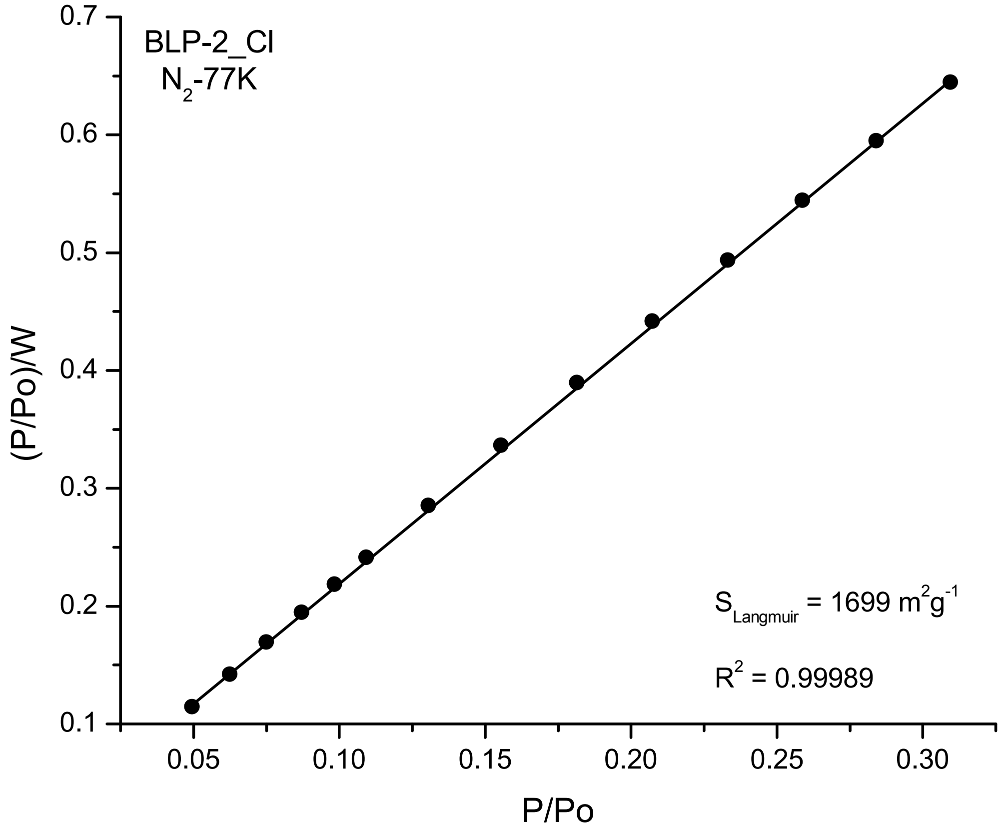


Figure S29: Multipoint BET plot for BLP-2(Cl) calculated from the nitrogen adsorption in the range 0.02-0.20 P/P$_o$.

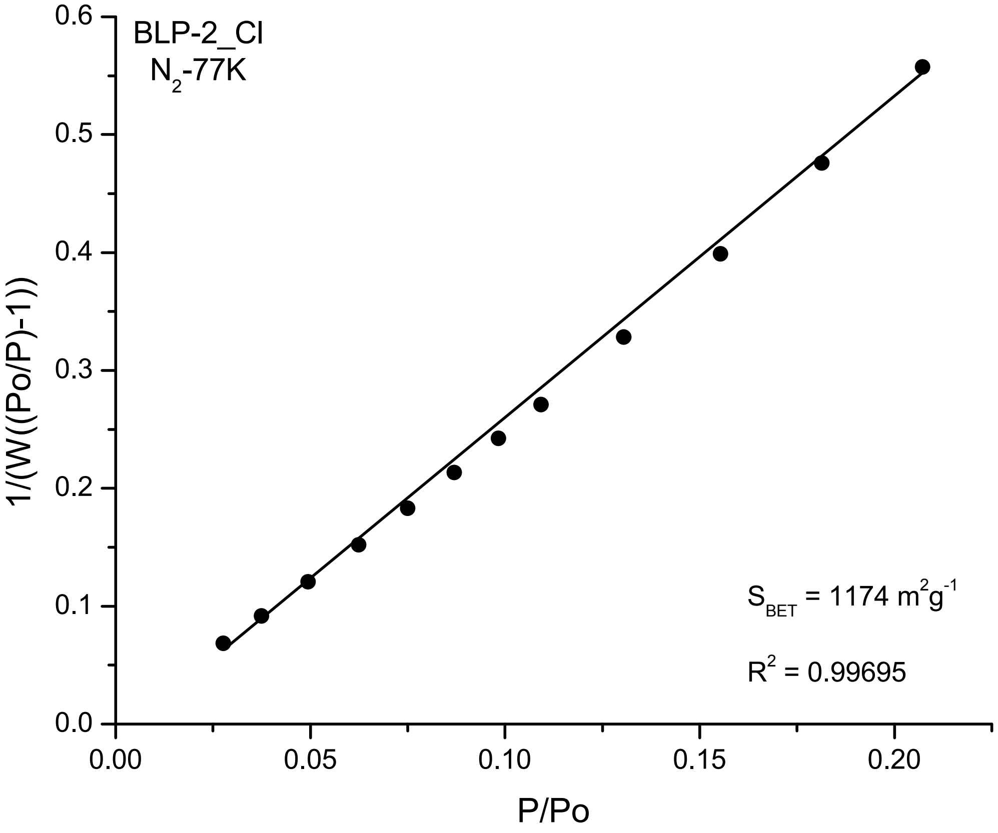


Table S1: Porous properties of all BLPs

Polymer	$SA_{Connolly}$[a] (m^2g^{-1})	SA_{Lang} (m^2g^{-1})	SA_{BET} (m^2g^{-1})	P_{vol} (cm^3g^{-1})	PSD (nm)	H_2 (wt%)
BLP-1(Cl)	1291	1828	1364	0.746	1.3	1.10
BLP-1(Br)	937	730	503	0.303	1.3	0.68
BLP-2(Cl)	1540	1699	1174	0.649	1.3	1.30
BLP-2(Br)	1230	1221	849	0.571	1.3	0.98

[a] Calculated using Materials Studio

Figure S30: Hydrogen isotherms for all BLPs measured at 77K.

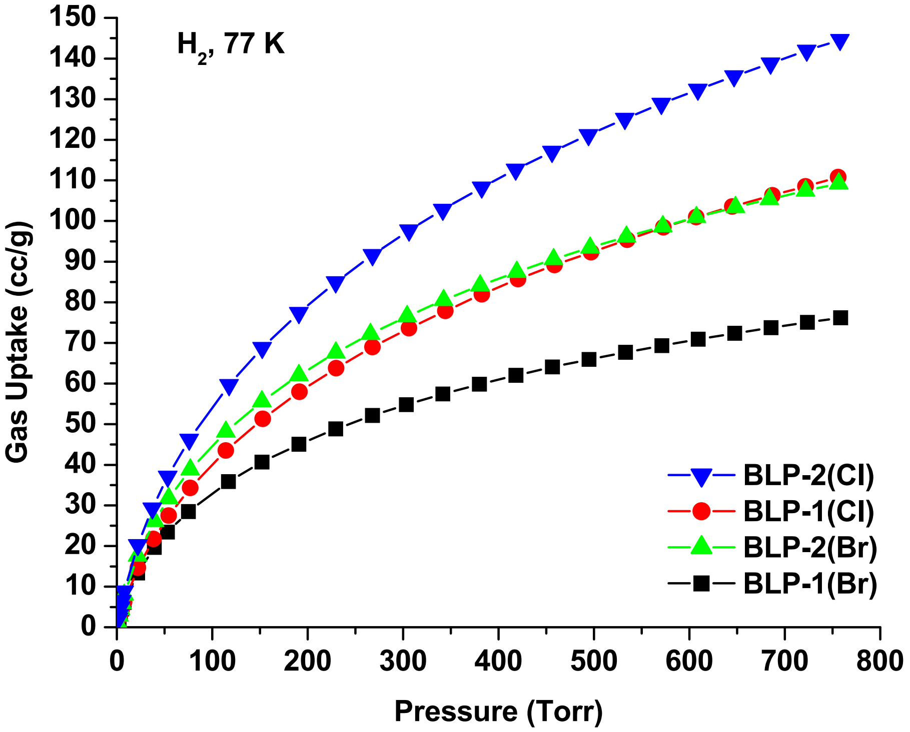


Figure S31: Hydrogen isotherms for all BLPs measured at 87K.

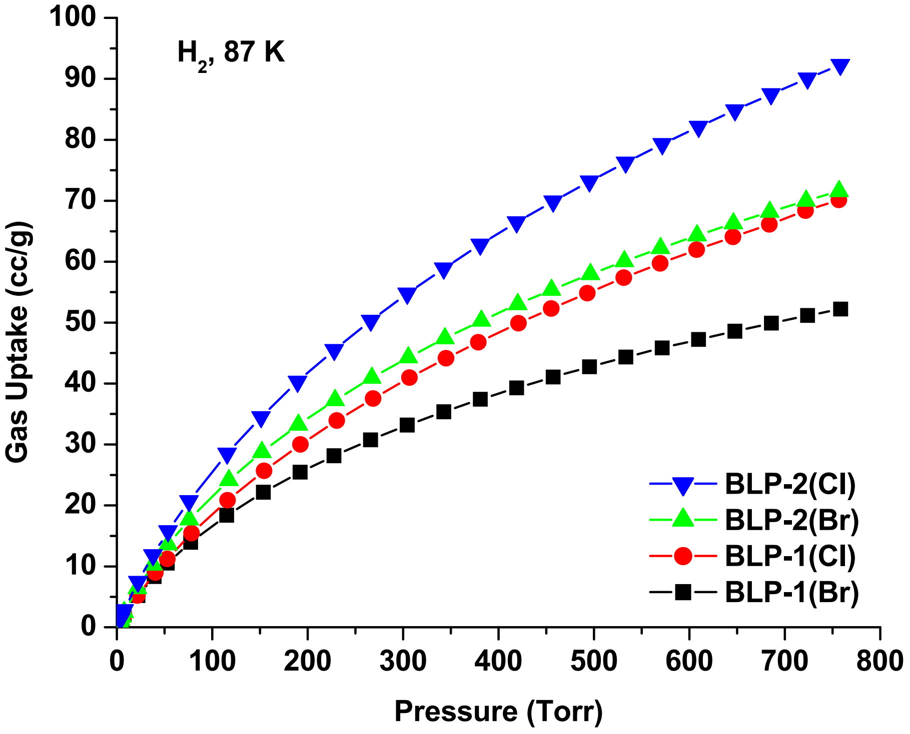


Figure S32. Carbon dioxide isotherm for BLP-1(Br) at 273 K.

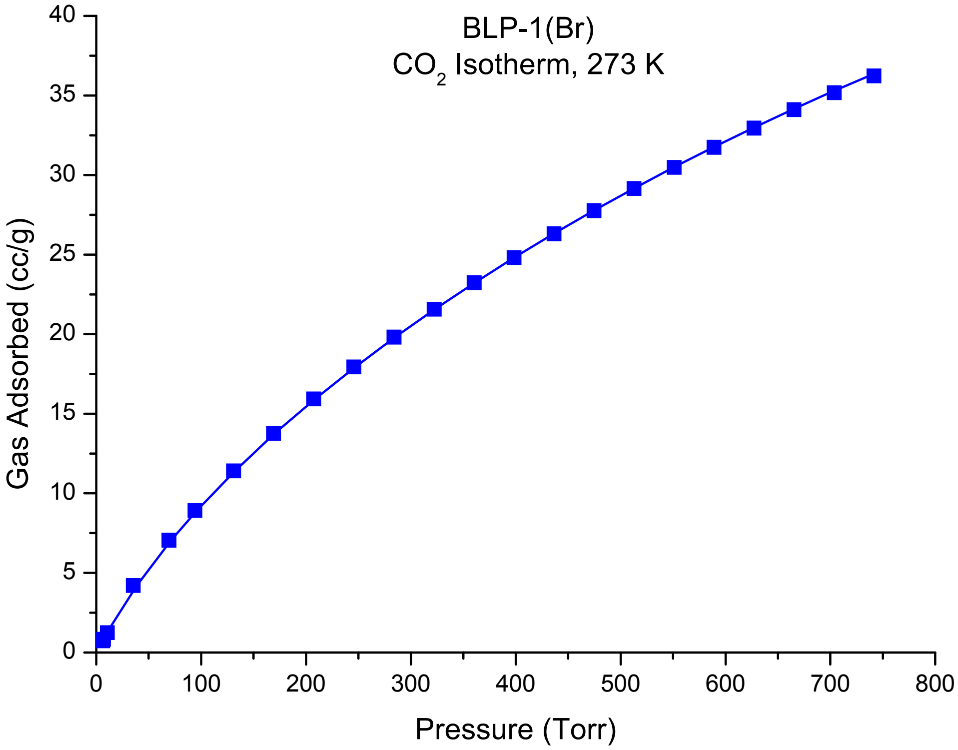


Figure S33. Carbon dioxide isotherm for BLP-1(Cl) at 273 K.

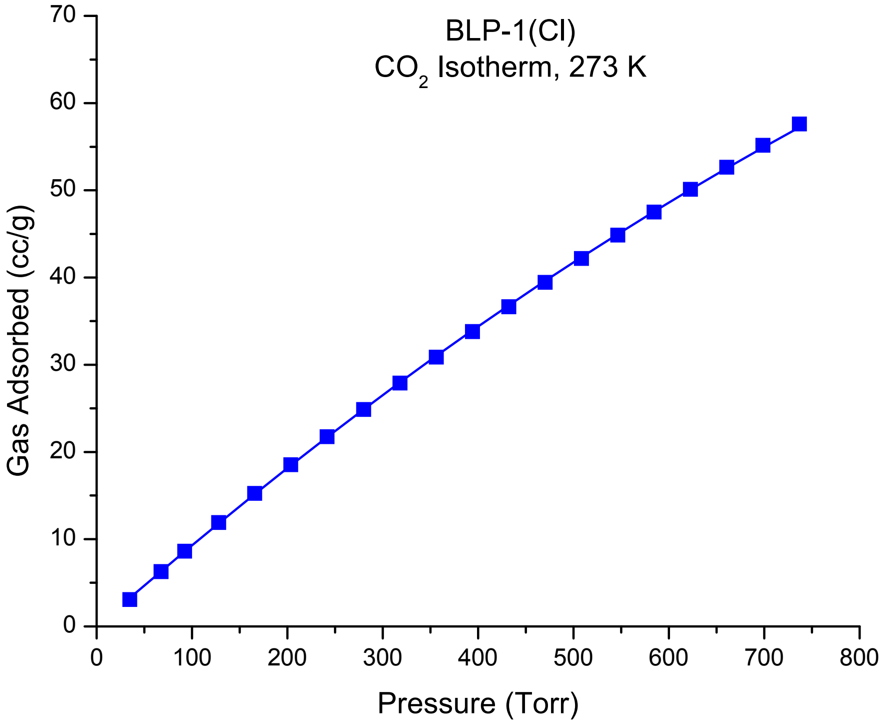


Figure S34. Carbon dioxide isotherm for BLP-2(Br) at 273 K.

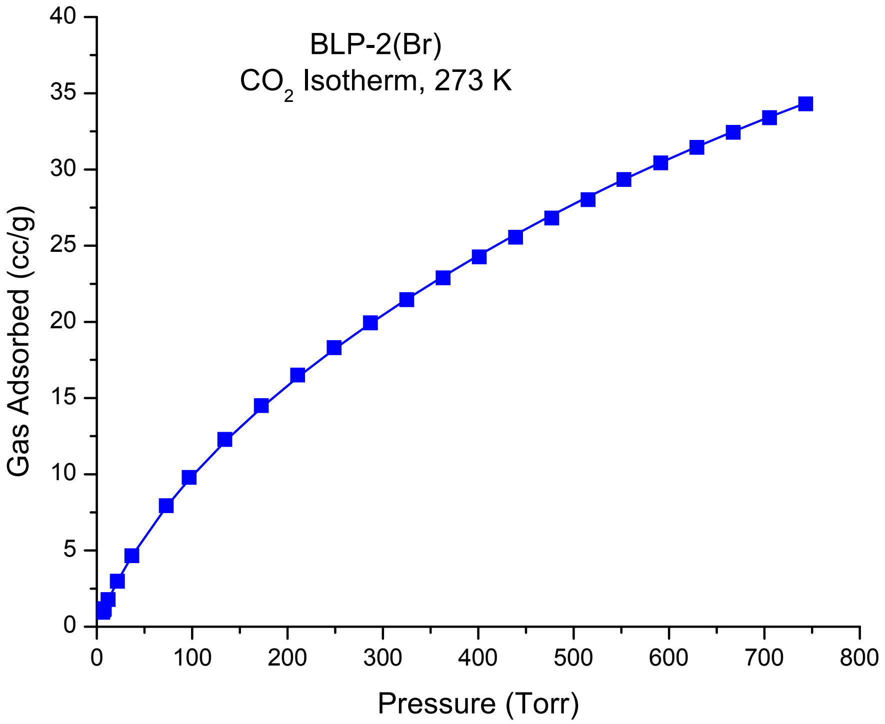
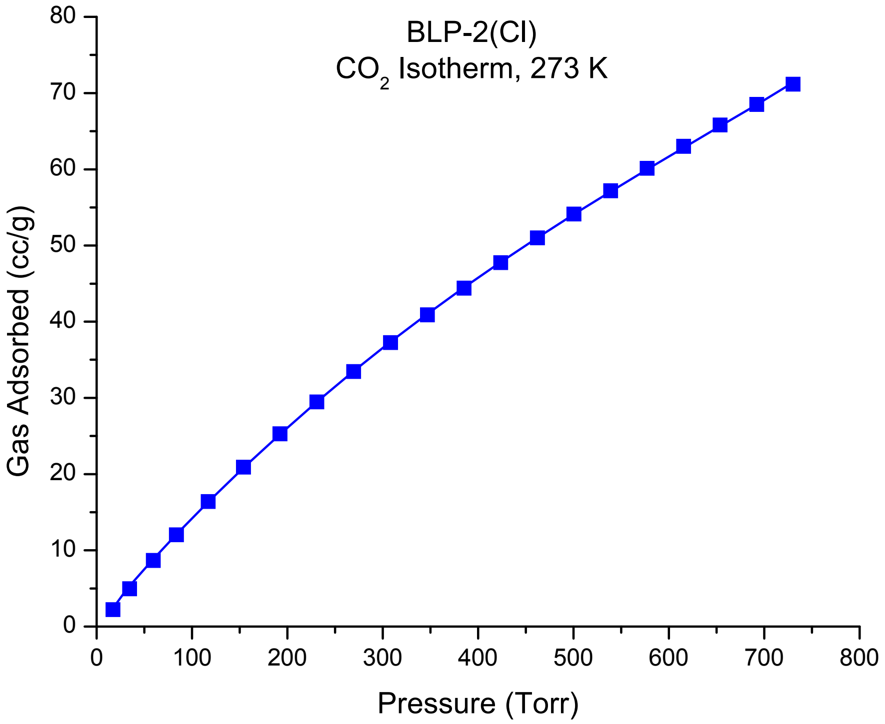


Figure S35. Carbon dioxide isotherm for BLP-2(Cl) at 273 K.



Section S7: *2D Borazine-Linked Polymer (BLP) Structural Models and Atomic Coordinates*

BLP-1(Br) and BLP-1(Cl) models were constructed using *Materials Studio Visualizer*[5]. Each polymer was modeled using boron nitride (**bnn**, P6/*mmm*) and graphite (**gra,** $P6_3/mmc$) topologies. Vertex positions were obtained from the Reticular Chemistry Structure Resource[6]. Dimensions of the unit cell were expanded beyond what any reasonable energetic minimization would result in to prevent overlapping of atoms. Subsequently, each vertex was replaced by a borazine ($B_3H_6N_3$) ring orientated such that the nitrogen atoms projected along the sites of extension. The hydrogen atoms attached to the nitrogen atoms were deleted whereas the hydrogen atoms attached to the boron atoms were replaced with the appropriate halide (bromine or chlorine). The midpoint of each extension was replaced by benzene and connected to the nitrogen atoms. The models were then optimized. BLP-2(Br) and BLP-2(Cl) models were also constructed using *Materials Studio Visualizer* in a similar fashion to BLP-1(Br) and BLP-1(Cl). Each polymer was modeled using a derivative form of the boron nitride topology with a space group of P-6*m*2 as well as using the graphite topology (**gra,** $P6_3/mmc$) as is. The dimensions of the unit cell were expanded as before. For the graphite topology, half of the vertices were replaced by a borazine orientated such that the nitrogen atoms projected along the sites of extension and the hydrogen atoms dealt with in a similar fashion to BLP-1(Br) and BLP-1(Cl). The other half of the vertices was replaced with a benzene ring. The midpoint of each extension was also replaced by a benzene ring. The carbon atom on this latter benzene ring closest to a nitrogen atom on the same plane was connected to this nitrogen atom; additionally, the para-carbon of the benzene ring was attached to the closest same plane benzene ring that functions as a vertex. The models were then optimized. For the boron nitride-derivative topology P-6*m*2 for BLP-2(Br) and BLP-2(Cl) following the unit cell expansion, half of the vertices were replaced by borazine with the nitrogen atoms functioning as the sites of extension, and the other half of the vertices were replaced with a benzene ring. The midpoint of each extension was again replaced by a benzene ring, and connections were made in a similar fashion to the graphite topology of BLP-2(Br) and BLP-2(Cl). The models were then optimized.

After constructing the models using *Materials Studio Visualizer* as described above, their geometry was optimized using the Vienna ab initio simulation package (VASP) and projector augmented wave (PAW) methods[7]. Calculations were carried out using local density approximation (LDA) based on the density functional theory (DFT). High precision calculations with a cutoff energy of 400 eV for the plane-wave basis were used. The Brillouin zone integration was carried out using the special Monkhorst-Pack sampling. The total energies were converged to below 0.1 meV. Gaussian smearing was applied for relaxing the geometry. The optimization was considered to be converged when the total force on the atoms was less than 5 meV/Å.

The positions of atoms in the unit cell for the modeled topologies were determined using *Diamond Version 3.1* and are shown as fractional atomic coordinates in Tables S2-S9.

Table S2: Fractional atomic coordinates for the eclipsed conformation of BLP-1(Br) calculated from *Materials Studio* modeling.

BLP-1(Br)

Boron Nitride

P6/mmm

a = b = 16.6630 Å ; c = 3.6529 Å
$\alpha = \beta = 90^{o}$; $\gamma = 120^{o}$

Atom	*x*	*y*	*z*
B1	0.2807	0.5615	0.0000
Br1	0.7857	0.2142	0.0000
C1	0.4077	0.4572	0.0000
C2	0.4449	0.5551	0.0000
H1	0.4074	0.0685	0.0000
N1	0.7806	0.3903	0.0000

Table S3: Fractional atomic coordinates for the staggered conformation of BLP-1(Br) calculated from *Materials Studio* modeling.

BLP-1(Br)			
Graphite $P6_3/mmc$ a = b = 15.7095 Å ; c = 6.8546 Å α = β = 90° ; γ = 120°			
Atom	*x*	*y*	*z*
B1	0.3893	0.6107	0.2500
B2	0.1118	0.0559	0.2500
Br1	0.4633	0.5367	0.2500
Br2	0.1298	0.2595	0.7500
C1	0.1126	0.2252	0.2500
C2	0.2207	0.4414	0.2500
C3	0.2153	0.2820	0.2500
C4	0.2666	0.3846	0.2500
H1	0.5720	0.6550	0.2500
H2	0.7690	0.7560	0.2500
N1	0.0576	0.1153	0.2500
N2	0.2756	0.5512	0.2500

Table S4: Fractional atomic coordinates for the eclipsed conformation of BLP-1(Cl) calculated from *Materials Studio* modeling.

BLP-1(Cl)

Boron Nitride

P6/mmm

a = b = 16.4547 Å ; c = 3.5878 Å
$\alpha = \beta = 90^{o}$; $\gamma = 120^{o}$

Atom	*x*	*y*	*z*
B1	0.2806	0.5612	0.0000
C1	0.4057	0.4555	0.0000
C2	0.4451	0.5549	0.0000
Cl1	0.7806	0.2194	0.0000
H1	0.4055	0.0706	0.0000
N1	0.7807	0.3903	0.0000

Table S5: Fractional atomic coordinates for the staggered conformation of BLP-1(Cl) calculated from *Materials Studio* modeling.

BLP-1(Cl)

Graphite

P6_3*/mmc*

a = b = 16.5011 Å ; c = 6.8643 Å
α = β = 90º ; γ = 120º

Atom	*x*	*y*	*z*
B1	0.3838	0.6162	0.2500
B2	0.1007	0.0504	0.2500
C1	0.1092	0.2183	0.2500
C2	0.2234	0.4467	0.2500
C3	0.2098	0.2819	0.2500
C4	0.2609	0.3836	0.2500
Cl1	0.4423	0.5577	0.2500
Cl2	0.1097	0.2195	0.7500
H1	0.5951	0.6675	0.2500
H2	0.7398	0.7405	0.2500
N1	0.0538	0.1076	0.2500
N2	0.2796	0.5591	0.2500

Table S6: Fractional atomic coordinates for the eclipsed conformation of BLP-2(Br) calculated from *Materials Studio* modeling.

BLP-2(Br)

Boron Nitride Derivative

P-6*m*2

a = b = 15.7273 Å ; c = 3.6481 Å
α = β = 90º ; γ = 120º

Atom	*x*	*y*	*z*
B1	0.4407	0.7204	0.0000
Br1	0.5783	0.7891	0.0000
C1	0.5654	0.2827	0.0000
C2	0.6145	0.2290	0.0000
C3	0.5532	0.5927	0.0000
C4	0.6054	0.5423	0.0000
C5	0.5590	0.4410	0.0000
C6	0.4481	0.5519	0.0000
H1	0.4120	0.3157	0.0000
H2	0.3365	0.3901	0.0000
H3	0.7558	0.5116	0.0000
N1	0.3901	0.6099	0.0000

Table S7: Fractional atomic coordinates for the staggered conformation of BLP-2(Br) calculated from *Materials Studio* modeling.

BLP-2(Br)

Graphite

$P6_3/mmc$

a = b = 15.5929 Å ; c = 7.1543 Å
α = β = 90º ; γ = 120º

Atom	*x*	*y*	*z*
B1	0.3836	0.6164	0.2500
Br1	0.4469	0.5530	0.2500
C1	0.0525	0.1050	0.2500
C2	0.1083	0.2166	0.2500
C3	0.2206	0.4412	0.2500
C4	0.1018	0.0509	0.2500
C5	0.2108	0.2716	0.2500
C6	0.2614	0.3753	0.2500
H1	0.0895	0.1791	0.7500
H2	0.6113	0.6666	0.2500
H3	0.7628	0.7434	0.2500
N1	0.2787	0.5575	0.2500

Table S8: Fractional atomic coordinates for the eclipsed conformation of BLP-2(Cl) calculated from *Materials Studio* modeling.

BLP-2(Cl)

Boron Nitride Derivative

P-6*m*2

a = b = 15.5253 Å ; c = 3.6681 Å
$\alpha = \beta = 90^{\circ}$; $\gamma = 120^{\circ}$

Atom	*x*	*y*	*z*
B1	0.4411	0.7206	0.0000
C1	0.5647	0.2824	0.0000
C2	0.6143	0.2286	0.0000
C3	0.5539	0.5946	0.0000
C4	0.6067	0.5441	0.0000
C5	0.5587	0.4413	0.0000
C6	0.4478	0.5522	0.0000
Cl1	0.5708	0.7854	0.0000
H1	0.4085	0.3131	0.0000
H2	0.3331	0.3898	0.0000
H3	0.7564	0.5129	0.0000
N1	0.3900	0.6100	0.0000

Table S9: Fractional atomic coordinates for the staggered conformation of BLP-2(Cl) calculated from *Materials Studio* modeling.

BLP-2(Cl)

Graphite

P6_3/*mmc*

a = b = 15.5267 Å ; c = 7.1876 Å
α = β = 90º ; γ = 120º

Atom	*x*	*y*	*z*
B1	0.3835	0.6165	0.2500
C1	0.0528	0.1056	0.2500
C2	0.1089	0.2179	0.2500
C3	0.2211	0.4422	0.2500
C4	0.1026	0.0513	0.2500
C5	0.2124	0.2730	0.2500
C6	0.2635	0.3774	0.2500
Cl1	0.4426	0.5574	0.2500
H1	0.0902	0.1804	0.7500
H2	0.6057	0.6627	0.2500
H3	0.7615	0.7412	0.2500
N1	0.2790	0.5580	0.2500

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