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Supplementary Information

Balancing Functional Properties and Environmental Impact of Graphitic Carbon Nitride: A Case Study on Boron Doping Syntheses

Yash Shah [a, c], Leanne M. Gilbertson [*a, b, c]

[a] Department of Civil and Environmental Engineering, University of Pittsburgh, Pittsburgh, USA – 15206

[b] Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, USA – 15206

[c] Department of Civil and Environmental Engineering, Duke University, Durham, USA – 27708

*Corresponding author: Leanne M. Gilbertson, leanne.gilbertson@duke.edu

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1. SAMPLE PREPARATION FOR ALL THE CHARACTERIZATION TECHNIQUES

1.1. X-Ray Diffraction (XRD). XRD patterns were collected on a Bruker D8 Discover instrument using Cu Ka radiation at a generator voltage of 40 kV and a generator current of 40 mA. The scan speed was 0.40 seconds/step, the step size was 0.02°, and the angle range was 10-60°.

1.2. Transmission Electron Microscopy (TEM). Electron microscopy imaging was obtained using a JEOL JEM-2100F transmission electron microscope operated at 200 kV. The TEM specimen was prepared by applying 10-20 mL suspensions of the BCN sample (100 mg mL^{-1}) in ethanol onto holey carbon films supported on Cu TEM grids.

1.3. X-ray Photoelectron Spectroscopy (XPS). Surface elemental composition of the BCN samples were evaluated by XPS. A Thermo Scientific ESCALAB 250Xi instrument (monochromatic Al Kα X-ray source, 1486.7 eV, spot size 650 μm) was employed to analyze the samples that were prepared by placing approximately 2 mg of powder BCN onto the sample holder covered with double-sided copper tape. A pass energy of 150 eV with a step size of 1.0 eV was used to obtain the survey spectra, and a pass energy of 50 eV with a step size of 0.1 eV was used to collect high-resolution B1s, C1s, and N1s spectra. For each sample, at least three measurements in different locations were carried out. The software Thermo Scientific Avantage was used to process the spectra in order to calculate the atomic percentage of elements, and to determine the distribution of B, C, and N species by peak deconvolution. For component-fitting of the spectra, each spectrum was subtracted with a modified Shirley background, and the C1s peak at 284.8 eV was used for energy scale correction.

1.4. Band gap determination. UV-Vis diffuse reflectance measurements were performed using the LAMBA-750 UV-Vis-NIR spectrophotometer (Perkin Elmer L750) equipped with a 60 mm integrating sphere. Measurements were collected over the wavelength range of 200 to 800 nm. The angle of incidence of the light beam on the sample was set to 0 degrees in order to exclude the specular reflectance contribution to the intended measurement of diffuse reflectance only. The reflectance data (R) obtained express the relative reflectance of the

sample compared to a barium sulfate ($BaSO_4$) standard. The spectra in percent reflectance were converted using the Kubelka-Munk function *F(R)*. For the measurements, BCN or BaSO4 powder was loaded into a powder holder (Perkin Elmer 52123164) until the quartz window was completely covered. Indirect optical band gap values were obtained from the Tauc plots, as well documented in the literature[1–3].

1.5. Steady-state Photoluminescence (ss-PL). The ss- PL of BCN in solution were obtained by using FluoroMax-3 (Jobin Yvon Horiba). BCN powder was dispersed in deionized water at a concentration of 0.25 mg mL^{-1}, and bath sonicated (VWR Aquasonic 150T) for 1 h. For ss-PL measurements, the emission spectra ranging from 345 to 640 nm wavelength was obtained at an excitation wavelength of 330 nm in a UV cuvette (4.5 mL, Fisher Scientific) under constant magnetic stirring. Since ss-PL depends on light absorbance of the photocatalysts, absorbance of BCN in solution was measured from the same aliquots used for ss-PL.

2. LCA INVENTORY DETAILS FOR BCN SYNTHESIS ROUTES

2.1. Supramolecular synthesis of 1 mmol S-BCN

Synthesis yield: 24.03%

LCI Details:

LCI Inputs

i. 1 g melamine
ii. 0.06 g boric acid
iii. 1.02 g cyanuric acid

The synthesis of cyanuric acid was created based on the procedures reported by She et al[4]. In detail, 20 g of urea was added to 40 mL of kerosene as solvent. The mixture was stirred at 150 °C, placed under vacuum, and then heated at 190 °C until the reaction was complete. The reaction mixture was cooled to 80 °C, put into 15 mL of water, and stirred for 1 hour to precipitate the product. The obtained dry solid was heated to 150 °C for 2 hours to remove the crystallization water and afford pure cyanuric acid. The synthesis yield of cyanuric acid is 89%.

Electricity calculations using the Thermo ScientificTM SP88854100 stirring hot plate with power consumption of 540 W:

i. Stirring: Assumed 3 h. 540 W × 3 h = 1.62 kWh
ii. Heating: Assumed 4 h. 540 W × 4 h = 2.16 kWh
iii. Stirring: 1 h. 540 W × 1 h = 0.54 kWh
iv. Drying: 2 h. 540 W × 2 h = 1.08 kWh

Total = (1.62 + 2.16 + 0.54 + 1.08) = 5.4 kWh

iv. 40 mL of ethanol, which is equal 31.56 g of ethanol (density of 0.789 g/mL)

v. Nitrogen gas: assuming flow of 100 mL/min, and temperature 21^0C for 6 h 10 min (370 min).

$$1 \text{ L/min} \times 370 \text{ min} \times 1.25 \text{ kg/m}^3 \times 1\text{m}^3/1000 \text{ L} = 0.04625 \text{ kg} = 46.25 \text{ g}$$

vi. Electricity (stirring): 3 h duration

- Considering the Thermo ScientificTM SP88854100 stirring hot plate with power consumption of 540 W

Electricity (sonication): 1 h duration

- Using the Aquasonic 150 HT bath sonicator with power consumption of 400 W

Electricity (drying): 16 h duration

- Assuming the Thermo ScientificTM SP88854100 stirring hot plate with power consumption of 540 W

Electricity (calcination): Calculated for a heating temperature of 500 °C for 3 h using a tube furnace, when the heating speed is 2.5 °C min^{-1}

- Assuming the Thermo Scientific Lindberg/Blue M TF55035A-1 tube furnace with power consumption of 800 W.

Electricity input calculations:

Total time of tube furnace turned on for heating:
Start temperature = 25 °C (room temperature)
Annealing temperature = 500 °C
Heating rate = 2.5 °C/min

Time to reach annealing temperature = (500 °C – 25 °C) / (2.5 °C/min) = 190 min = 3.17 h. Total time of furnace turned on = 3.17 h + 3 h = 6.17 h

Electricity consumed = Device power consumption (W) × time of use (h)

- Stirring = 540 W × 3 h = 1.62 kWh
- Bath sonication = 400 W × 1 h = 0.4 kWh
- Drying (hot plate) = 540 W × 16 h = 8.64 kWh
- Calcination (tube furnace) = 800 W × 6.17 h = 4.94 kWh

Total = (1.62 + 0.4 + 8.64 + 4.94) kWh = 15.6 kWh

LCI Emissions to Air

0.27 g of Ammonia

1.02 g of Cyanic acid

31.56 g Ethanol

46.25 g of Nitrogen

Table S1. Life cycle inventory to produce BCN using the supramolecular method, including the Pedigree matrix for unit processes (all distributions assumed to be lognormal).

	Section	Material	Amount	Unit	LCI Database	Pedigree Matrix SD[2]	Comments
1 g of 1 mmol S BCN	Input	Melamine	1.00	g	Melamine (GLO) | market for | Cut-off, U	1, 4, 1, 1, 1, na 1.11	
		Ethanol	43.55	g	Ethanol, from ethylene (RoW) | market for ethanol | Cut-off, U	1, 4, 1, 1, 1, na 1.11	
		Boric Acid	0.06	g	Boric acid, anhydrous, powder (GLO) | market for | Cut-off, U	1, 4, 2, 3, 1, na 1.12	
		Cyanuric Acid	1.02	g	Based on [4]	1, 4, 1, 1, 1, na 1.11	Based on [4]
		Nitrogen	46.25	kg	Nitrogen, atmospheric	2, 4, 1, 1, 1, na 1.12	Calcination inert gas
		Electricity	16	kWh	Electricity, at grid, US/US	4, 4, 1, 1, ,1 , na 1.24	Used for stirring, sonication, drying, and calcination

	Emission to air	Ammonia	0.27	g		2, 4, 5, 1, 1, na 1.53	Approximately 2 NH_3 liberated by melamine pyrolysis at 550 °C for 4h (mole/mole melamine). Based on [5,6] $C_3H_6N_6 \rightarrow g\text{-}C_3N_4 + 2\ NH_3$
		Ethanol	43.55	g		1, 4, 1, 1, 1, na 1.11	Evaporation
		Isocyanic acid	1.02	g		2, 4, 5, 1, 1, na 1.53	All cyanuric acid is decomposed into cyanic acid at 550 °C. Based on [7,8] $(CNOH)_3\ (s) \rightarrow 3\ HNCO\ (g)$
		Nitrogen	46.25	g		2, 4, 1, 1, 1, na 1.12	Calcination inert gas

Table S2. User-defined life cycle inventory to produce cyanuric acid [4,9], including the Pedigree matrix for unit processes (all distributions assumed to be lognormal).

Section	Material	Amount	Unit	LCI Database	Pedigree Matrix SD^2	Comments
Cyanuric Acid (for 12.75 g)	Urea	9.2	g	Urea, as N, at regional storehouse/US-US-EI/U US-EI	1,4,4,3,1,na 1.24	This LCI refers to 1 kg of N, resp. 2.17 kg urea with a N-content of 46%. Thus, to account for the 20 g of urea needed, the amount of 9.2 g is used
Yield 89% Based on [4]	Kerosene	40	mL	Kerosene, at refinery/I/US USLCI	1,4,4,3,1,na 1.24	
	Deionized water	15	g	Water, deionised, at plant/US* US-EI U US-EI	1,4,4,3,1,na 1.24	

		Electricity	5.4	kWh	Electricity mix 2018/US U US-EI	4,4,1,1,1,na 1.24	Used for stirring, heating, drying
	Emission to air	Ammonia	5.67	g		1,4,4,3,1,na 1.24	3 $CH_4N_2O \rightarrow (CNOH)_3 + 3\ NH_3$ Based on [10]
		Water	15	g		1,4,4,3,1,na 1.24	Evaporation

2.2. Synthesis of 1 mmol NS-BCN-BA:

Synthesis yield: 61.30%

LCI Details:

LCI Inputs

i. 1 g melamine

ii. 0.06 g boric acid

iii. 10 mL of deionized water

iv. Air gas: assuming flow of 100 mL/min, and temperature 21^0C for 5.75 h (345 min).

$$1\ \text{L/min} \times 345\ \text{min} \times 1.2\ \text{kg/m}^3 \times 1\text{m}^3/1000\ \text{L} = 0.0414\ \text{kg} = 41.4\ \text{g}$$

v. Electricity (stirring): 3 h duration

- Considering the Thermo ScientificTM SP88854100 stirring hot plate with power consumption of 540 W

Electricity (drying): 16 h duration

- Assuming the Thermo ScientificTM SP88854100 stirring hot plate with power consumption of 540 W

Electricity (calcination): Calculated for a heating temperature of 550 °C for 4 h using a tube furnace, when the heating speed is 5 °C min^{-1}

- Assuming the Thermo Scientific Lindberg/Blue M TF55035A-1 tube furnace with power consumption of 800 W.

Electricity input calculations:

Total time of tube furnace turned on for heating:

Start temperature = 25 °C (room temperature)

Annealing temperature = 550 °C

Heating rate = 5 °C/min

Time to reach annealing temperature = (550 °C – 25 °C) / (5 °C/min) = 105 min = 1.75 h. Total time of furnace turned on = 1.75 h + 4 h = 5.75 h

Electricity consumed = Device power consumption (W) × time of use (h)

- Stirring = 540 W × 3 h = 1.62 kWh
- Drying (hot plate) = 540 W × 16 h = 8.64 kWh
- Calcination (tube furnace) = 800 W × 5.75 h = 4.6 kWh

Total = (1.62 + 8.64 + 4.6) kWh = 14.86 kWh

LCI Emissions to Air

0.27 g of Ammonia

10 g water

41.4 g of air

Table S3. Life cycle inventory to produce NSBCN-BA, including the Pedigree matrix for unit processes (all distributions assumed to be lognormal).

	Section	Material	Amount	Unit	LCI Database	Pedigree Matrix SD[2]	Comments
1 g of 1 mmol NS BCN BA	Input	Melamine	1.00	g	Melamine (GLO) | market for | Cut-off, U	1, 4, 2, 1, 1, na 1.12	
		Water	40.00	g	Water, deionized (RoW) |water production, deionized | Cut-off, U	1, 4, 4, 3, 1, na 1.24	
		Boric Acid	0.06	g	Boric acid, anhydrous, powder (GLO) | market for | Cut-off, U	1, 4, 2, 3, 1, na 1.12	
		Electricity	14.86	kWh	Electricity, at grid, US/US	4,4,1,1,1,na 1.24	Used for stirring, drying, and calcination
	Emission to air	Ammonia	0.27	g		1,4,4,3,1,na 1.24	Approximately 2 NH_3 liberated by melamine pyrolysis at 550 °C for 4h

					(mole/mole melamine). Based on [6] $C_3H_6N_6 \rightarrow g\text{-}C_3N_4 + 2\ NH_3$
	Water	40	g	1, 4, 4, 3, 1, na 1.24	Evaporation

2.3. Synthesis of 0.64 mmol NS-BCN-AB:

Synthesis yield: 21.78%

LCI Details:

LCI Inputs

i. 2 g dimethylacetamide. Since dicyandiamide was unavailable at the time of this study in either of the SimaPro libraries, it was assumed to be equivalent to dimethylacetamide, as assumed in a previous study[11].

ii. 0.02 g ammonia borane

The synthesis of ammonia borane was created as per the process described in a patent by Autrey et al.[12] The synthesis description is as follows: anhydrous NH_3 (10 mL) was condensed in an oven-dried 100 mL 3-neck round bottom flask fitted with a stir bar. The flask was cooled in a dry-ice/isopropanol bath (-78° C.) and opened to a nitrogen atmosphere. NH_4Cl (1.06 g, 18.6 mmol) and $NaBH_4$ (0.71 g, 18.6 mmol) were added by solids addition funnel to the three-neck flask, and the reaction was stirred for 2 hours under nitrogen at -78° C. Anhydrous tetrahydrofuran (THF) (100 mL) was slowly added dropwise to the flask via addition funnel, and NH_3 and H_2 were allowed to evaporate while thawing the reaction to room temperature and then stirred for another hour. Precipitated NaC1 was filtered away through filter paper. THF was then removed by rotary evaporation, followed by drying under a vacuum overnight. 0.58 g of the AB product [NH_3BH_3] was recovered as a microcrystalline powder (18.4 mmol, 99% yield).
Following the above procedure, the inputs in SimaPro were:

a. Anhydrous NH_3 = 0.0073 g (calculated using density = 0.73 kg/m^3 and 10 mL volume)
b. Ammonium chloride (NH_4Cl) = 1.06 g
c. Sodium tetrahydridoborate ($NaBH_4$) = 0.71 g
d. Tetrahydrofuran (THF) = 88.8 g (calculated using density = 0.888 kg/m^3 and for 100 mL volume)

e. Isopropanol = 339.7 g (calculated using the submerged volume of the three-neck flask to be 432.2 mL and density of isopropanol = 0.786 g/mL)

f. Nitrogen (liquid) = 349.2 g (calculated using the submerged volume of the three-neck flask to be 432.2 mL and density of isopropanol = 0.808 g/mL)

g. Electricity consumption:

- Stirring for 3 h = 3 h x 10 W = 0.03 kWh
- Rotary evaporator for 12 h = 12 h x 100 W = 1.2 kWh
- Vacuum drying for 12 h = 12 h x 180 W = 2.16 kWh

iii. 10 mL of deionized water

iv. N2 gas: assuming flow of 100 mL/min, and temperature 21^0C for 8 h (480 min).

$$1 \text{ L/min} \times 480 \text{ min} \times 1.25 \text{ kg/m}^3 \times 1\text{m}^3/1000 \text{ L} = 0.06 \text{ kg} = 60 \text{ g}$$

v. Electricity (stirring): 1 h duration

- Considering the Thermo ScientificTM SP88854100 stirring hot plate with power consumption of 540 W

Electricity (drying): 12 h duration

- Assuming the Thermo ScientificTM SP88854100 stirring hot plate with power consumption of 540 W

Electricity (calcination): Calculated for a heating temperature of 600 °C for 4 h using a tube furnace, when the heating speed is 2.39 °C min^{-1}

- Assuming the Thermo Scientific Lindberg/Blue M TF55035A-1 tube furnace with power consumption of 800 W.

Electricity input calculations:

Total time of tube furnace turned on for heating:
Start temperature = 25 °C (room temperature)
Annealing temperature = 600 °C
Heating rate = 5 °C/min
Time to reach annealing temperature = (600 °C – 25 °C) / (2.39 °C/min) = 240 min = 4 h. Total time of furnace turned on = 4 h + 4 h = 8 h
Electricity consumed = Device power consumption (W) × time of use (h)

- Stirring = 540 W × 1 h = 0.54 kWh
- Drying (hot plate) = 540 W × 12 h = 6.48 kWh

- Calcination (tube furnace) = 800 W × 8 h = 6.4 kWh

Total = (1.62 + 8.64 + 4.6) kWh = 13.42 kWh

LCI Emissions to Air

0.54 g Ammonia

60 g Nitrogen

10 g water

Table S4. Life cycle inventory to produce NSBCN-AB, including the Pedigree matrix for unit processes (all distributions assumed to be lognormal).

	Section	Material	Amount	Unit	LCI Database	Pedigree Matrix SD^2	Comments
1 g of 0.64 mmol NS BCN AB	Input	Dimethylacetamide	2.00	g	Dimethylacetamide (GLO) | market for | Cut-off, U	2, 4, 1, 1, 4, na 1.53	
		Ammonia Borane	0.02	g	Based on (add ref.)	3, 4, 4, 1, 1, na 1.26	
		Water	10	g	Water, deionized (RoW) |water production, deionized | Cut-off, U	1, 4, 4, 3, 1, na 1.24	
		Nitrogen	60	kg	Nitrogen, atmospheric	2, 4, 1, 1, 1, na 1.12	Calcination inert gas
		Electricity	11.98	kWh	Electricity, at grid, US/US	4,4,1,1, 1,na 1.24	Used for stirring, drying, and calcination
	Emission to air	Ammonia	0.54	g		5, 4, na, 1, 4, na 1.79	Assuming $C_2H_4N_4 \rightarrow (2/3)C_3N_4 + (4/3)NH_3$
		Water	10	g		1, 4, 4, 3, 1, na 1.24	Evaporation
		Nitrogen	60	kg		2, 4, 1, 1, 1, na 1.12	

Table S5. User-defined life cycle inventory to produce ammonia borane, including the Pedigree matrix for unit processes (all distributions assumed to be lognormal).

	Section	Material	Amount	Unit	LCI Database	Pedigree Matrix SD^2	Comments
Ammonia Borane	Input	Ammonia	0.0073	g	Ammonia, anhydrous, liquid {RoW}| market for ammonia, anhydrous, liquid | Cut-off, S	1, 4, 4, 3, 1, na 1.24	
		Ammonium chloride	1.06	g	Ammonium chloride {GLO}| market for | Cut-off, S	1, 4, 4, 3, 1, na 1.24	
		Sodium tetrahydridoborate	0.71	g	Sodium tetrahydridoborate {GLO}| market for | Cut-off, S	1, 4, 4, 3, 1, na 1.24	
		Tetrahydrofuran	88.8	kg	Tetrahydrofuran {GLO}| market for | Cut-off, S	1, 4, 4, 3, 1, na 1.24	
		Isopropanol	339.7	kWh	Isopropanol {RoW}| market for isopropanol | Cut-off, S	1, 4, 4, 3, 1, na 1.24	
		Nitrogen	349.2	g	Nitrogen, liquid {RoW}| market for | Cut-off, S	2, 4, 1, 1, 1, na 1.12	
		Electricity	2.49	kWh	Electricity, at grid, US/US	4,4,1,1,1, na 1.24	
	Emissions to air	Hydrogen	0.0236	g	Hydrogen	2, 4, 1, 1, 4, na 1.53	Assumed to evolve from anhydrous NH_3 and ammonium chloride NH_4Cl.
		Nitrogen, atmospheric	0.01694	g	Nitrogen, atmospheric	2, 4, 1, 1, 4, na 1.53	Assumed to evolve from anhydrous NH_3 and ammonium

3. UNCERTAINTY PLOTS FOR THE THREE BCN SYNTHESIS ROUTES

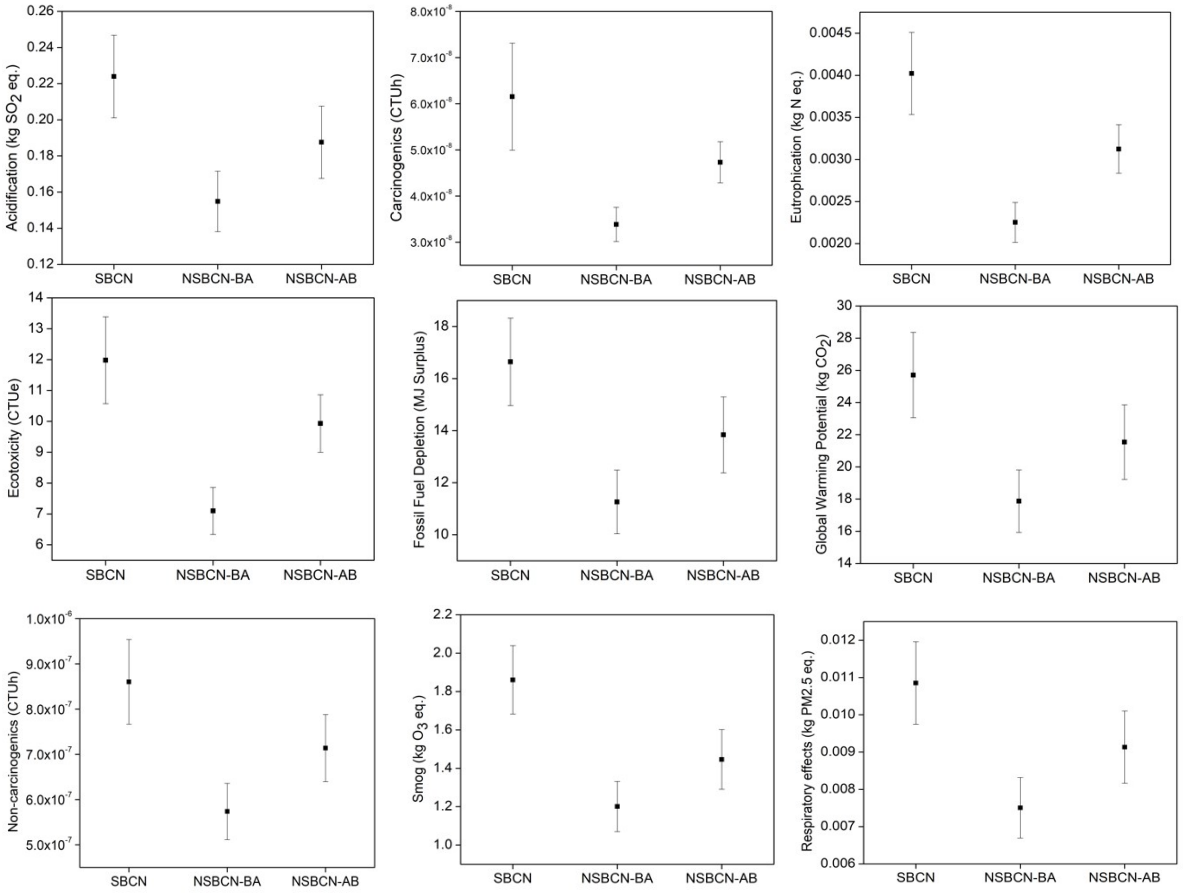


Figure S1. The mean impact and the associated uncertainty for each synthesis route in all assessed impact categories. Error bars represent standard deviation for the uncertainties in the unit processes and are calculated using a Monte Carlo approach.

4. XPS SPECTRA OF ALL THE SYNTHESIZED BCN SAMPLES IN THIS WORK

Table S6. B1s, C1s, and N1s XPS spectra for all the SBCN samples

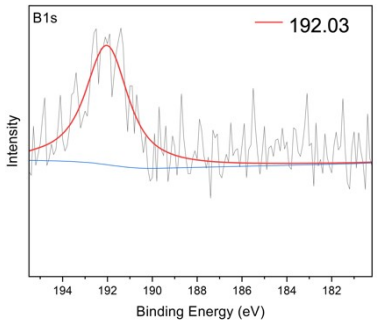
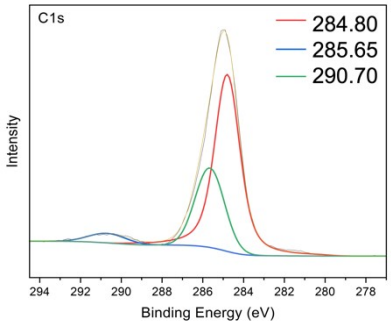
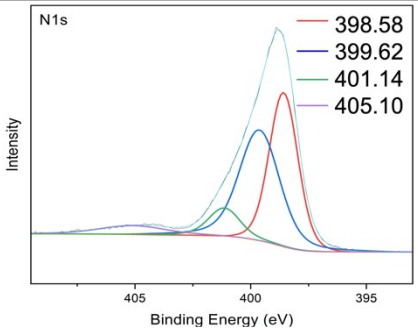
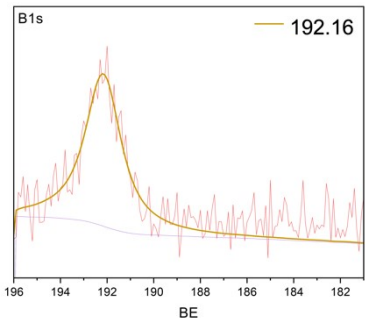
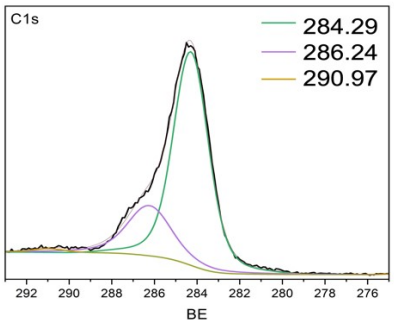
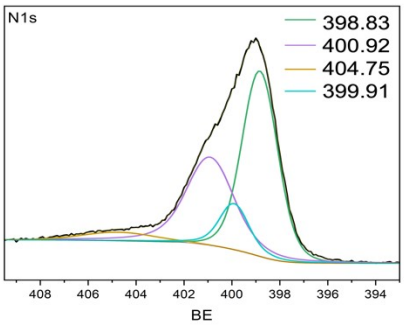
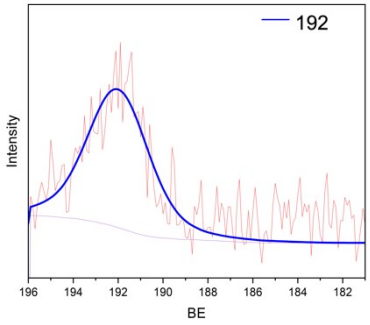
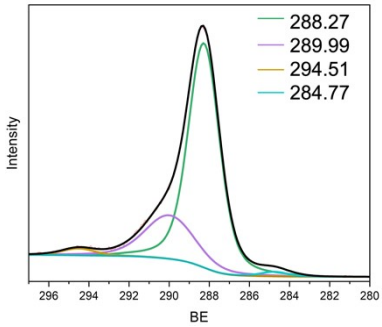
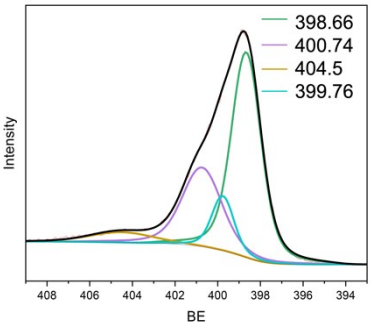
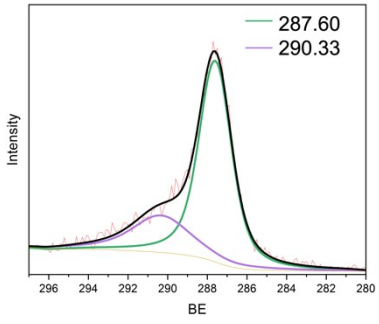
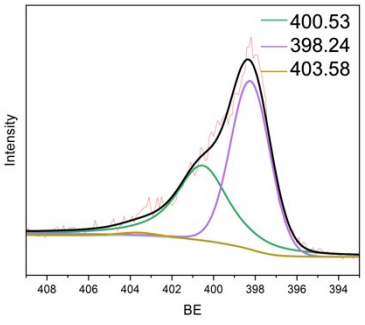
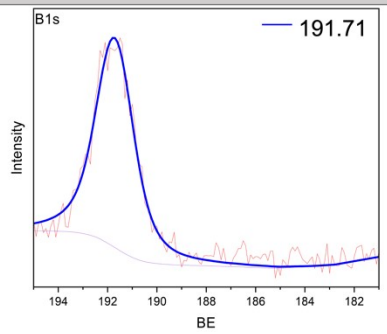
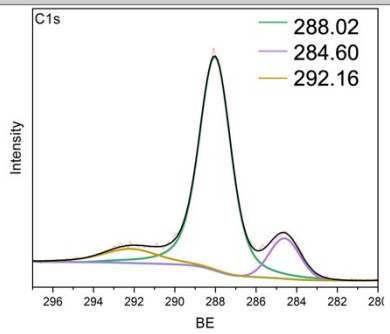
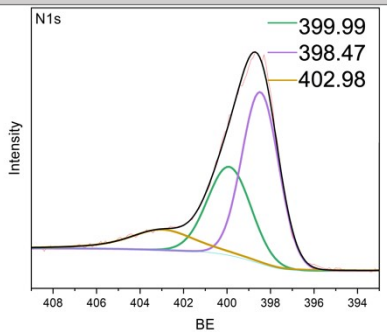
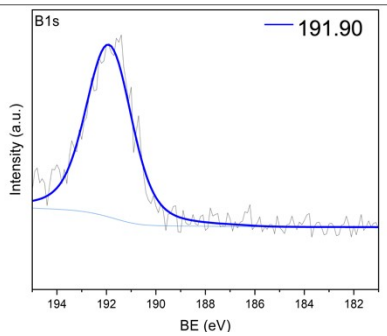
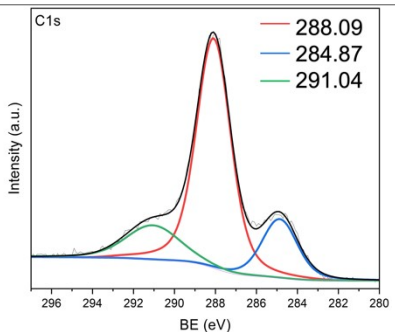
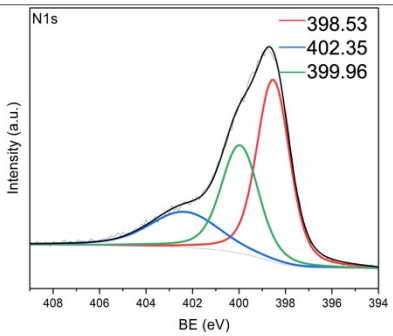
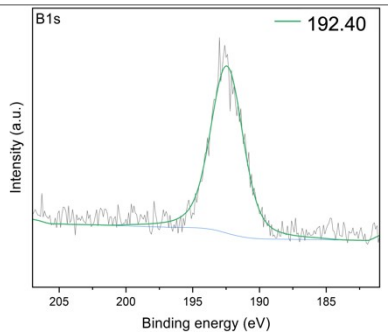
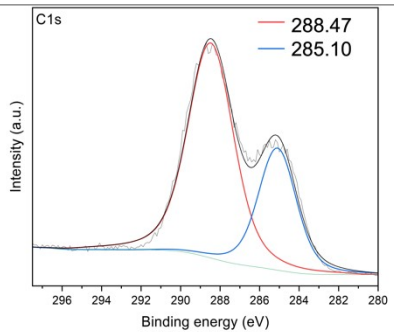
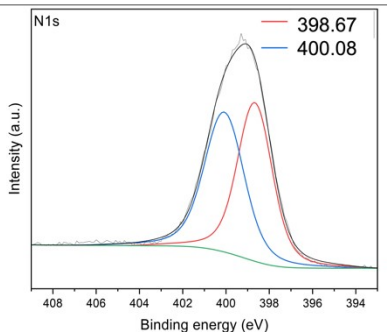
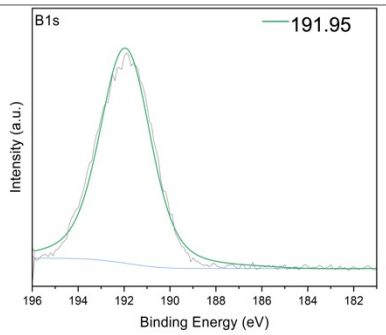
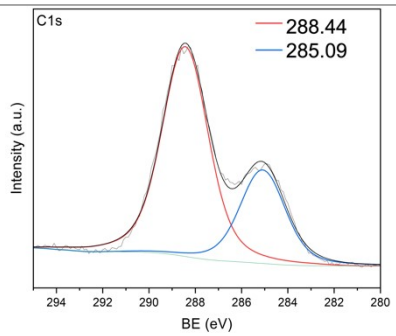
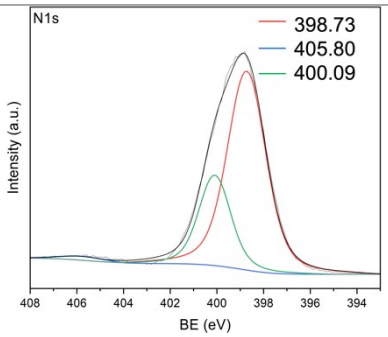
SBCN Sample	XPS		
	B1s	**C1s**	**N1s**
1 mmol BCN			
2 mmol BCN			
3 mmol BCN			
0 mmol BCN			

Table S7. B1s, C1s, and N1s XPS spectra for all the NSBCN-BA samples

NSBCNBA Sample	XPS		
	B1s	**C1s**	**N1s**
1 mmol BCN			
2 mmol BCN			
3 mmol BCN			
6 mmol BCN			

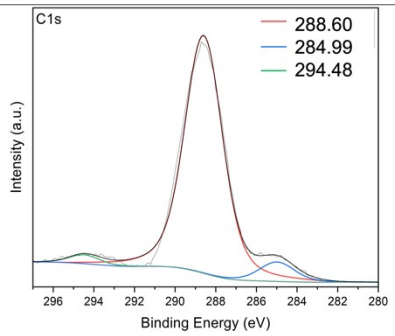
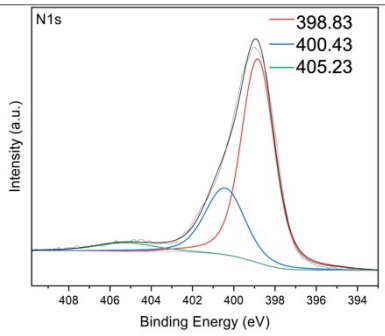
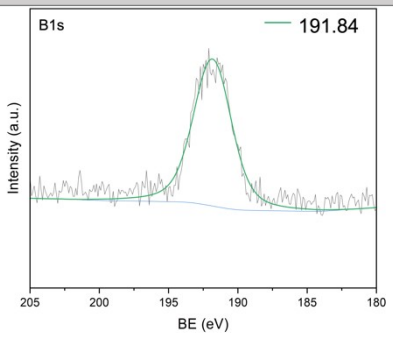
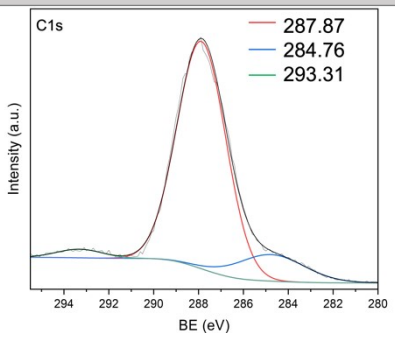
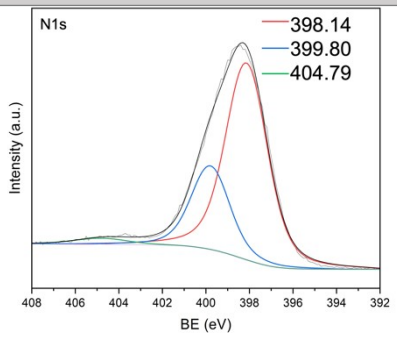
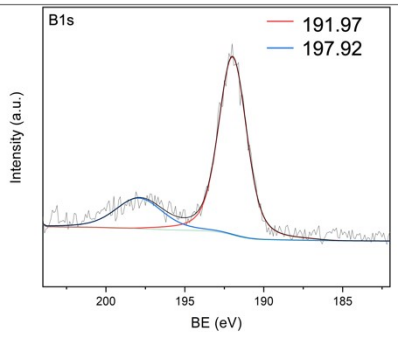
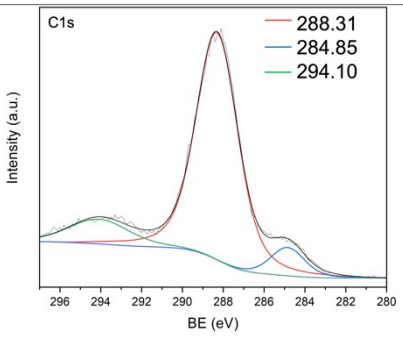
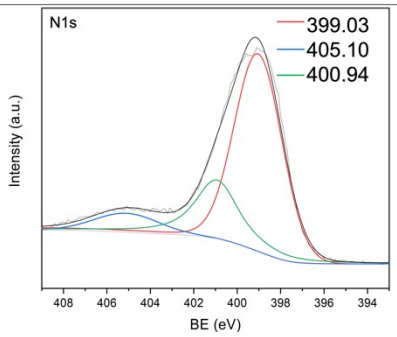
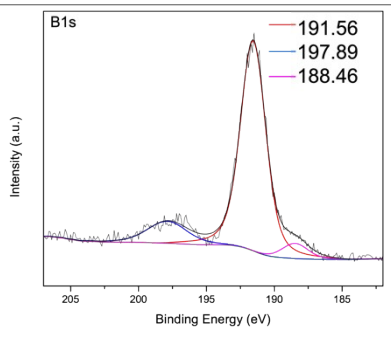
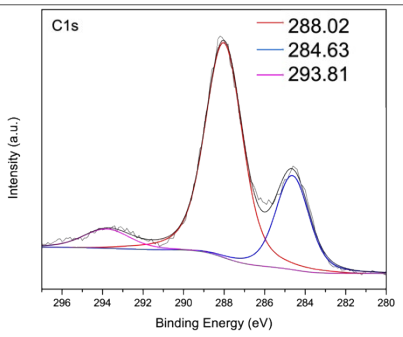
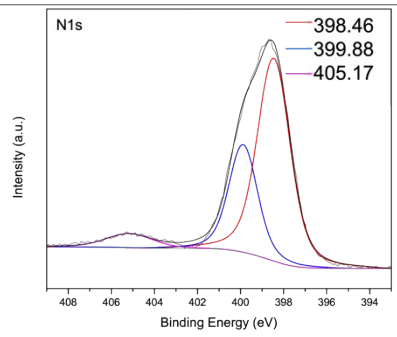
0 mmol BCN			

Table S8. B1s, C1s, and N1s XPS spectra for all the NSBCN-AB samples

NSBCNAB Sample	**XPS**		
	B1s	**C1s**	**N1s**
0.64 mmol BCN			
3.20 mmol BCN			
6.40 mmol BCN			

5. TAUC PLOTS MEASURING OPTICAL BANDGAPS OF BCN SAMPLES

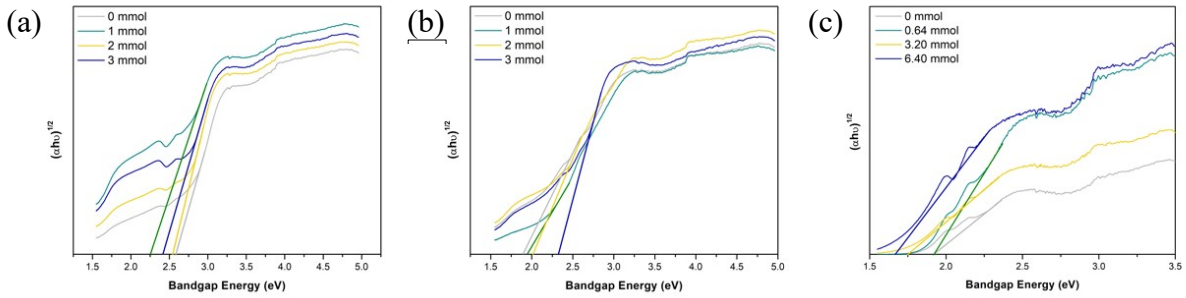


Figure S2. Tauc plots to measure bandgap for (a) SBCN; (b) NSBCN-BA; (c) NSBCN-AB samples. Bandgap is obtained using the x-axis intercept of the tangents drawn to the Tauc plot curve for each sample.

6. METHOD TO NORMALIZE ASSUMED UNITS FOR PHOTOLUMINESCENCE INTENSITIES FOR MAPS PLOTS

The metric of normalized assumed units for plotting on MAPS plots was generated using a simple method of measuring the PL intensities across PL plots and normalizing each PL intensity with the highest measured intensity in that sample set. For instance, in the NSBCN-BA PL plot (**Figure S3**), the normalized units for every sample were calculated as follows:

1. 0 mmol = (a) /(a) = 1592000/1592000 = 1.00
2. 1 mmol = (b)/(a) = 1276000/1592000 = 0.80
3. 2 mmol = (c)/(a) = 1178000/1592000 = 0.74
4. 3 mmol = (d)/(a) = 973000/1592000 = 0.61

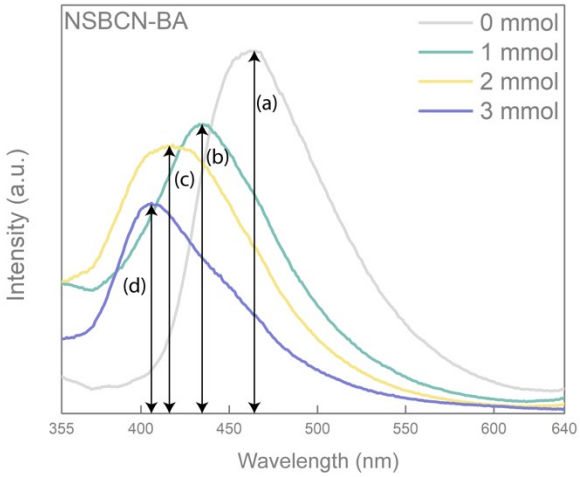


Figure S3. NSBCN-BA PL plot demonstrating the method to normalize assumed units for MAPS plots.

7. TRADEOFFS BETWEEN THE PHYSICOCHEMICAL PROPERTIES AND A FEW OTHER ENVIRONMENTAL IMPACT CATEGORIES

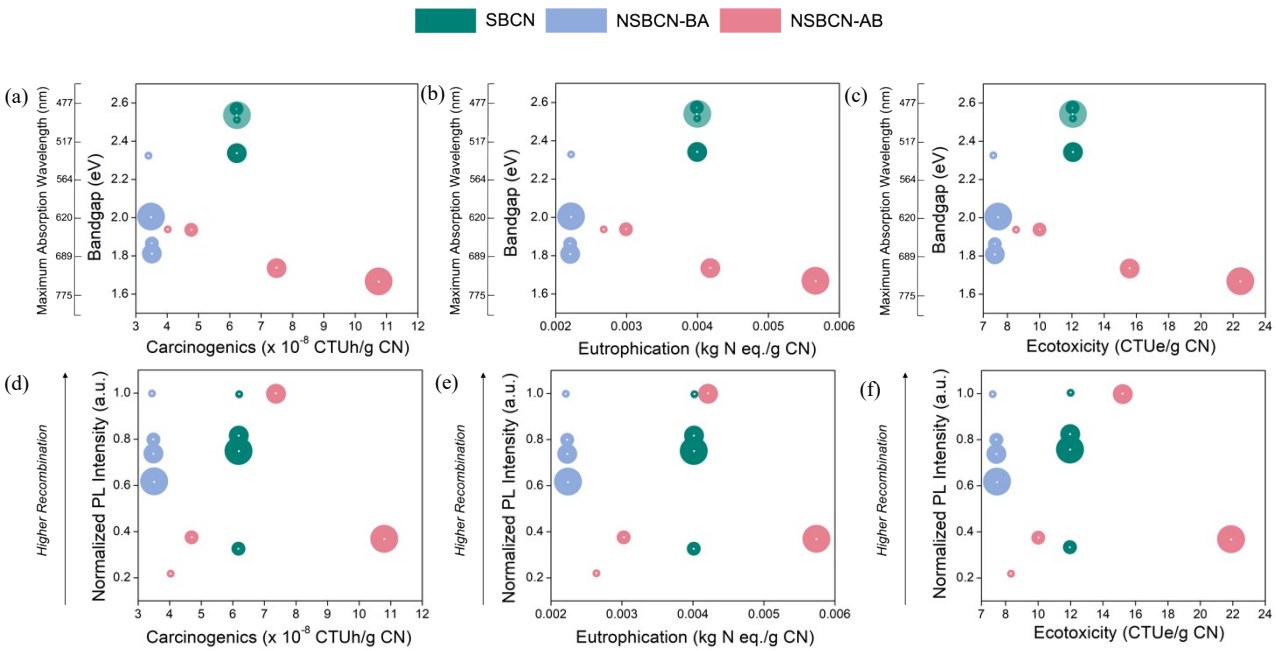


Figure S4. MAPS plots to analyze tradeoffs between optical bandgap and every BCN synthesis method's (a) carcinogenics, (b) eutrophication, (c) ecotoxicity. Similarly, for photoluminescence intensity and (d) carcinogenics, (e) eutrophication, (f) ecotoxicity. Size of colored dots is proportional to the heteroatom doping %. The size of the colored circles is proportional to the boron atomic % dopant. The center white dots represent the data point associated with the x-y coordinates.

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