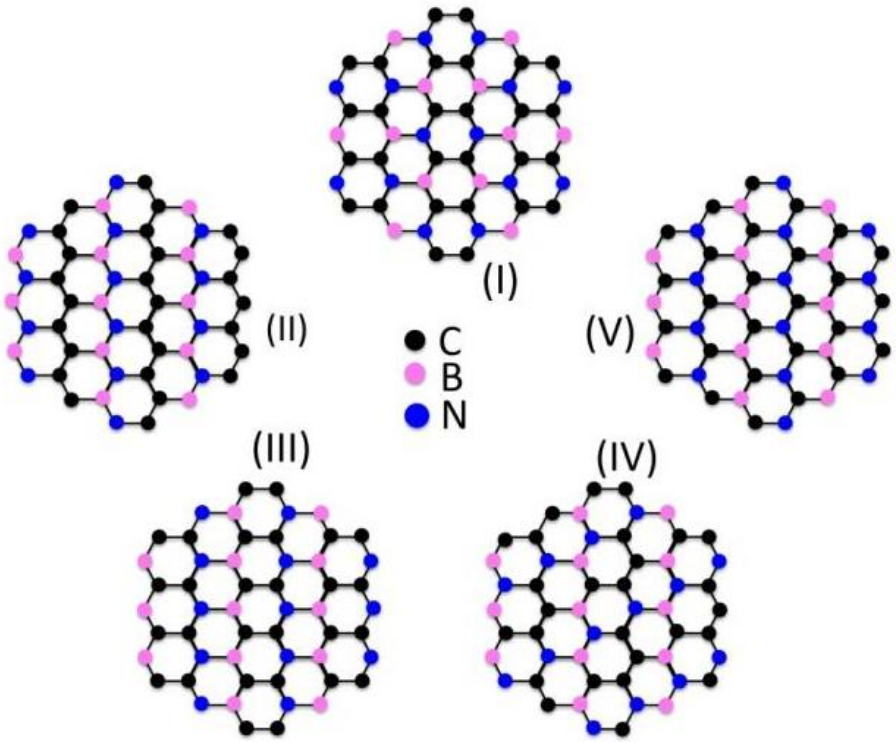
Boron Carbon Nitride (BCN)
A “new” 2D material



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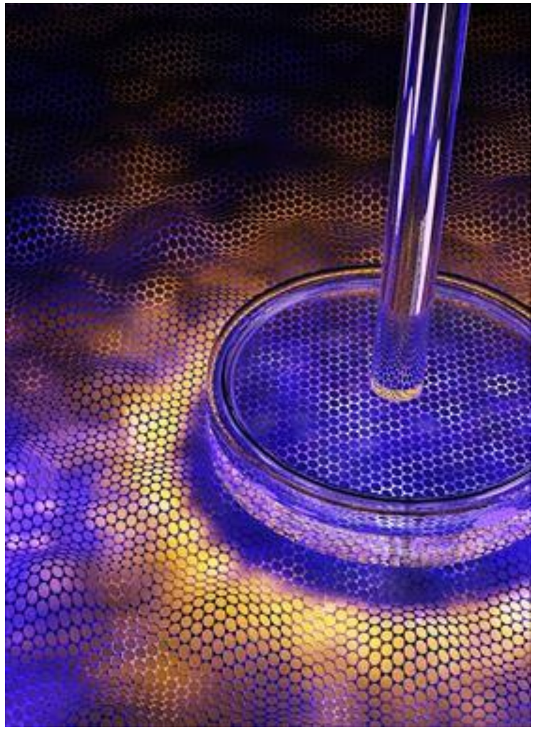
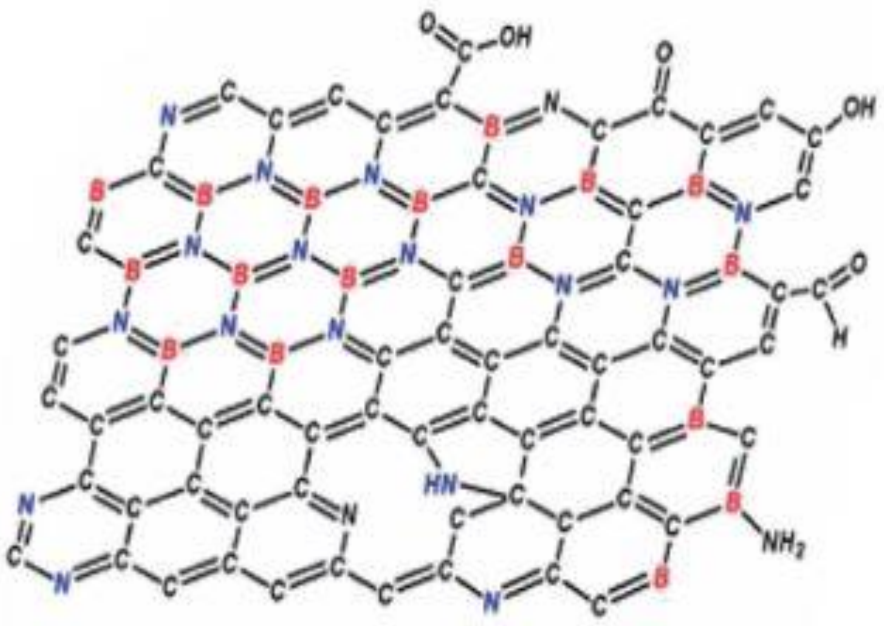
Introduction

- Boron carbon nitride (BCN) is a layered material with a structure similar to graphite and an interplanar distance of 0.349 nm, in which boron and nitrogen occupy the same positions of carbon.
- BCN can be imagined as an intermediate material between graphite and boron nitride, and can been obtained in nanosheets exhibiting interesting properties.



By compressing layers of boron nitride and graphene, researchers were able to enhance graphene's band gap **Image: Philip Krantz.**



Structure and Synthesis

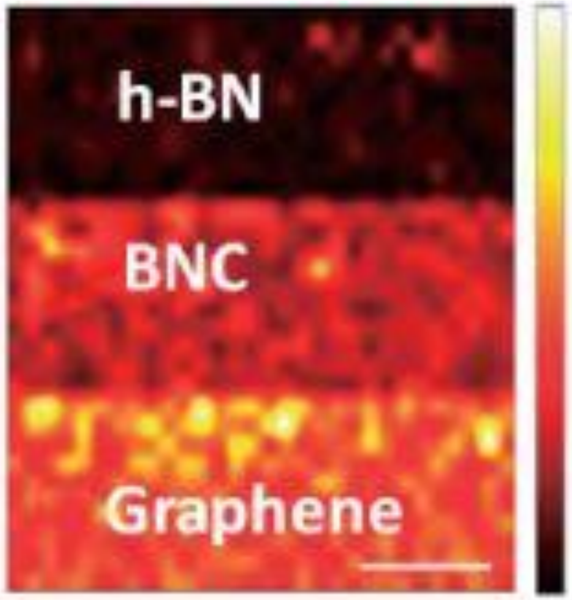
- Combustion reactions: From Boric Acid (source for Boron) and Urea (as a source for Nitrogen).
- Heteroepitaxial Growth. BCN hybrid nanosheets are also obtained by heteroepitaxial growth, two-step patching growth, where either graphene or BN nanosheet islands are first grown on the substrate; the other material is then patched onto the uncovered surface.
- Also made by CVD and Exfoliation processes

$$2H_3BO_3 \xrightarrow{\Delta} B_2O_3 + 3H_2O$$

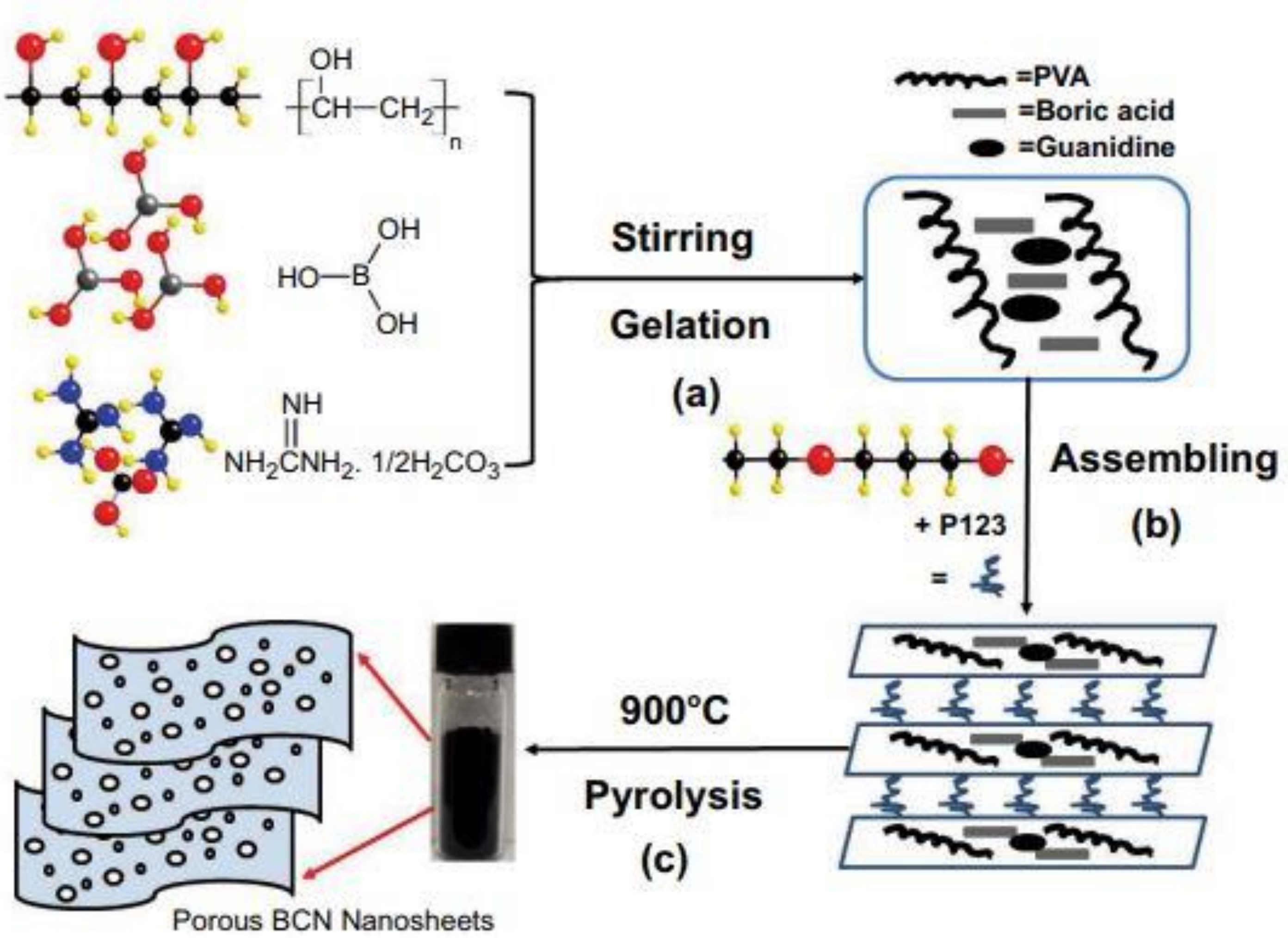
$$CO(NH_2)_2 \xrightarrow{\Delta} NH_3 + HNCO$$

$$B_2O_3 + 2NH_3 + 2C \xrightarrow{\Delta} 2BCN + 3H_2O$$

$$B_2O_3 + 2NH_3 + 4C \xrightarrow{\Delta} 2BC_2N + 3H_2O$$



Pluronic **P123**) symmetric triblock copolymer

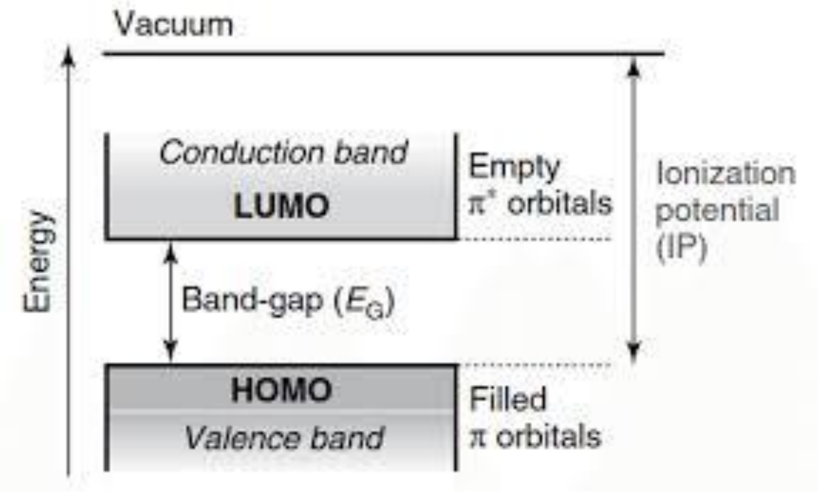


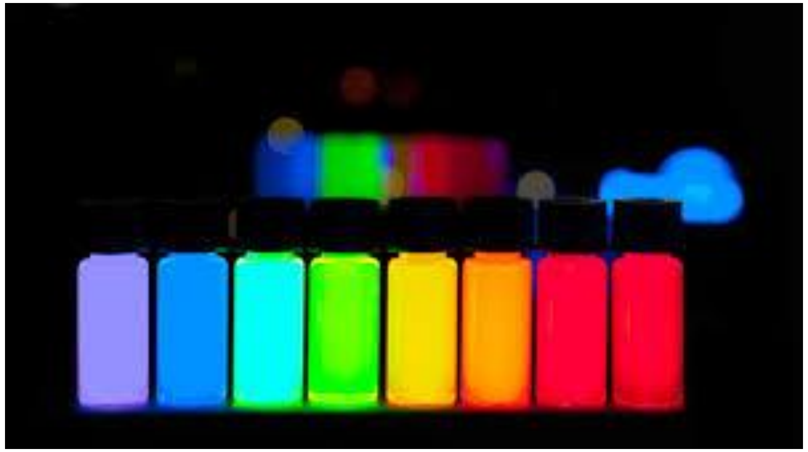
Scheme 2. Schematic synthesis process of porous BCN nanosheets including: (**a**) The gelation of polymer precursor. (**b**) The adding of P123 and (**c**) The pyrolysis at 900°C under N_2 [3].

Properties

- BCN is an organic semiconductor with a tunable band gap energy Eg: between 1 to 5 eV depending on the content of both nitrogen and carbon.

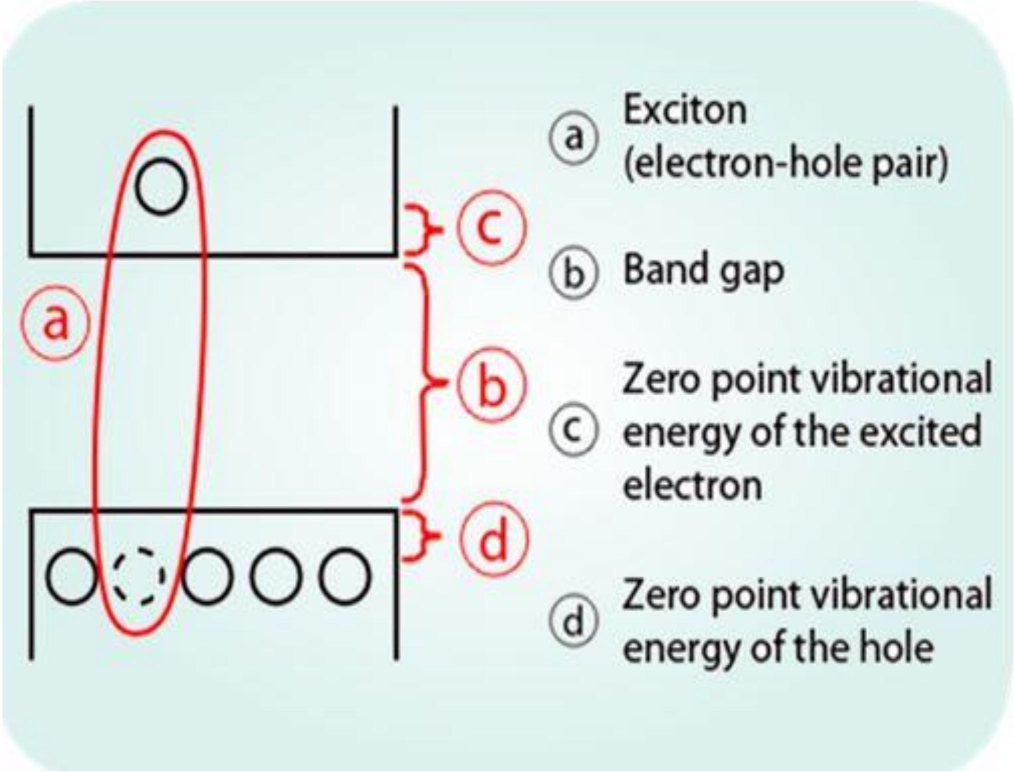
- As a consequence of the tunable Eg, BCN exhibits also a tunable photoluminescence that makes it interesting to be used to obtain quantum dots.





Properties (Continued)

- In semiconductors, light absorption generally leads to an electron being excited from the valence to the conduction band, leaving behind a hole.
- The electron and the hole can bind to each other to form an exciton. When this exciton recombines (i.e. the electron resumes its ground state), the exciton energy can be emitted as light (Fluorescence).
- As Metal free catalysts in electrochemical applications for HER, ORR reactions



The change in Band Gap upon substitution of Boron and Nitride in Graphene shows its extreme importance in electronic properties of materials.

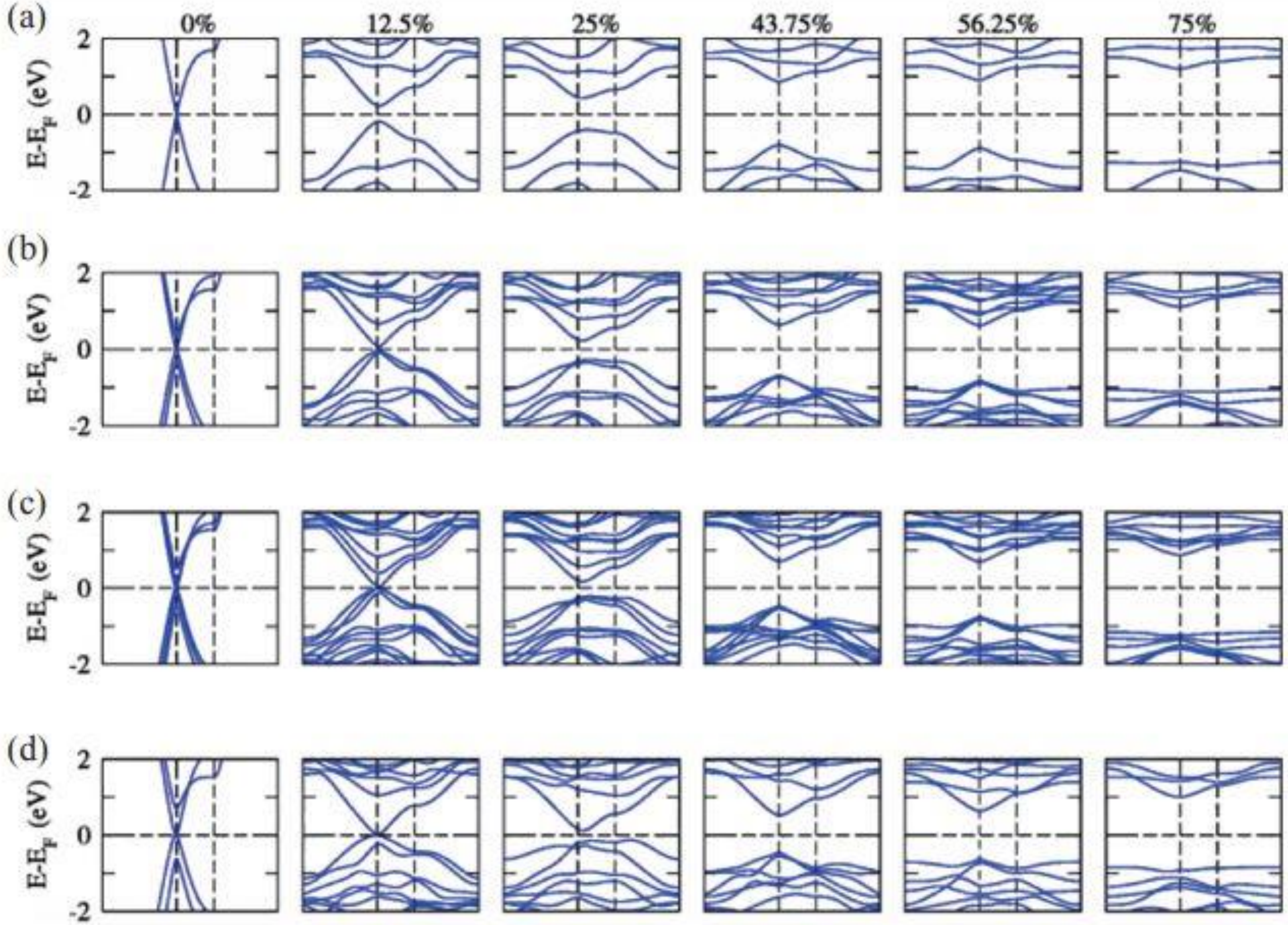


Figure 11. Electronic band structure of BN-substituted graphene for (a) mono (b) bi (c) tri and (d) multi-layer for concentrations between 0% and 75% (reproduced from ref. 45).

Applications of BCN nanomaterials

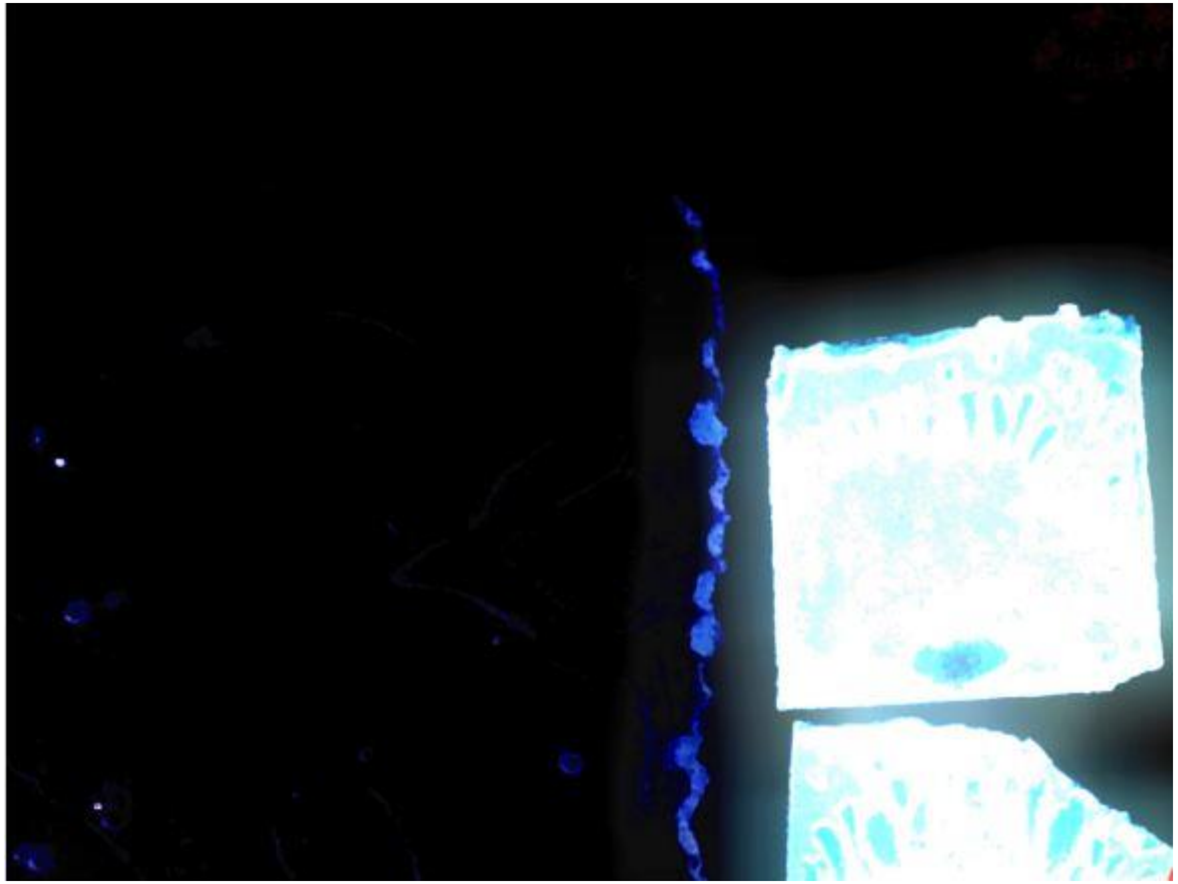
- Photocatalyst to oxidize contaminants and colorants
- Photocatalyst to produce hydrogen from water (instead of using Pt catalyst)
- Transparent photovoltaic cells (for buildings and cars)
- UV-absorber; Supramolecular Chemistry
- Catalyst to specific organic reactions
- Organic semiconductor to optoelectronics
- Fire retardant
- Phosphor to lighting applications and electronic screens
- Fluorescent material
- Supercapacitors

Categories	Nanomaterials	Applications
0D BCN	Nanospheres	CO_2 uptake
1D BCN	Nanotubes, nanoribbons, nanorods	ORR, supercapacitor
2D BCN	Nanosheets	ORR,HER, supercapacitor, lithium battery
3D BCN	Foams, aerogel	Gas adsorption

Property seen in an Application

The image on the right shows the fluorescence under a UV light due to the introduction of the 0.1 wt% of BCNO nanosheets into a poly methyl methacrylate (PMMA) matrix (right side) to be compared with a laminate of PMMA without fillers (left side).

BCN materials always contain a certain amount of oxygen in hydroxyl groups that allow the interaction with polar groups and make possible bonding to several materials. For this reason, they are sometimes indicated as BCNO



Challenges and Opportunities

- DFT Calculations and Simulations need to be used to optimize concentrations and orientations while developing the BxCyNz material. Determining the optimum x,y,z values for specific applications is the challenge.
- There are unlimited possibilities of ratios that have not been tried. There is huge scope for creating new layered materials.
- Ternary bonding formation of B,C,N is difficult to control and tune in an accurate way.
- There is a compromise between the high surface area and electro conductivity for porous BCN nanomaterials in energy applications. (As porous BCN have more defects, amorphous phases and asymmetry which reduces electro conductivity.
- Advanced modes of AFM can be used for characterization (Finding frictional coefficient, work function, topography etc)

References

- Dynamic band-structure tuning of graphene moiré superlattices with pressure: Yankowitz et. al. *Nature* volume 557, pages404–408 (2018)
- Boron Carbon Nitride (BCN) Nanomaterials: Structures, Synthesis and Energy Applications: Wang et. al. Current Graphene Science, 2018
- Borocarbonitrides, BxCyNz, 2D Nanocomposites with Novel Properties: **C. N. R. Rao** and K. Pramoda; Bull. Chem. Soc. Jpn. 2019
- https://www.materialstoday.com/nanomaterials/news/squeezing-a-band-gap-out-of-graphene/
- https://www.2dto3dmaterials.com/boron-carbon-nitride/

The End

- Thank you
- Questions ?
- This is the basis for my summer project (3 months) this year.
- I aim to make new inroads on this material.
- A lot of learning and reading and experimenting is left to do !