Synthesis of Ternary $B_xC_yN_z$ Compounds from Thermolysis of 1,2 – Diamineborane

towards hybrid BCN monolayer

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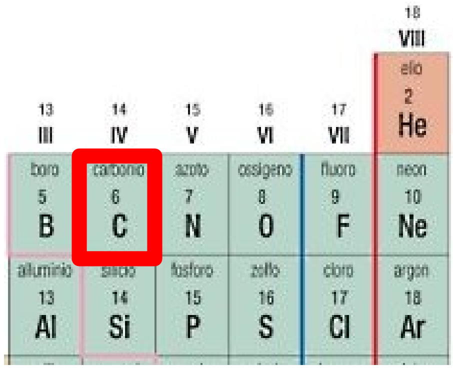
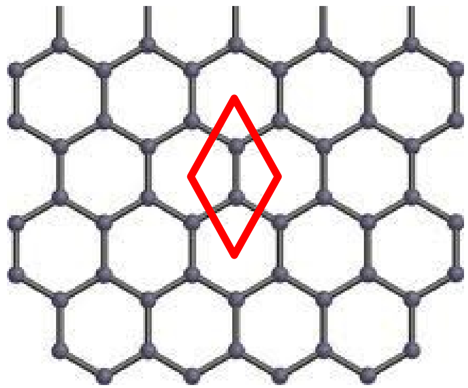
Fabrice Leardini
Dpto. De Fisica de Materiales M-04, Facultad de Ciencias, Universidad Autonoma de Madrid

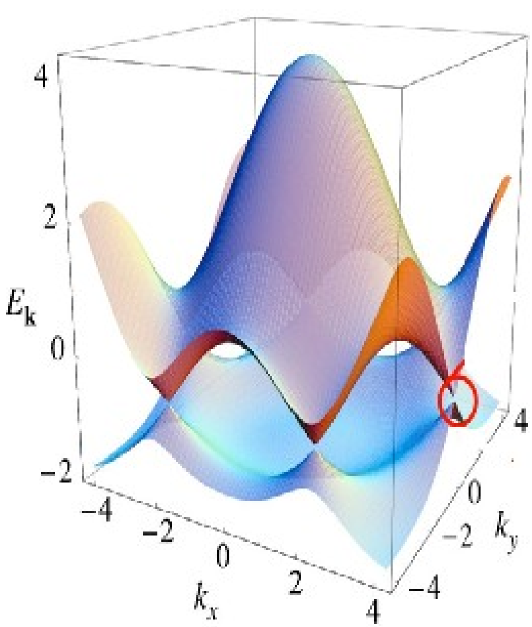
101° SIF meeting, Roma 21-25 September

Graphene vs h-BN



Graphene



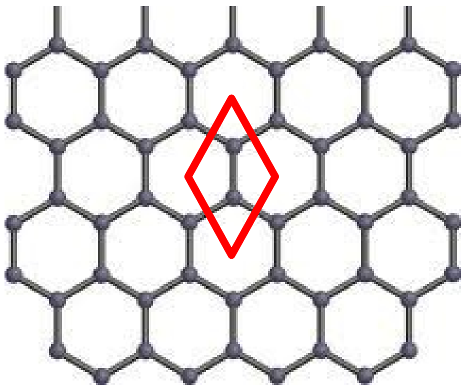


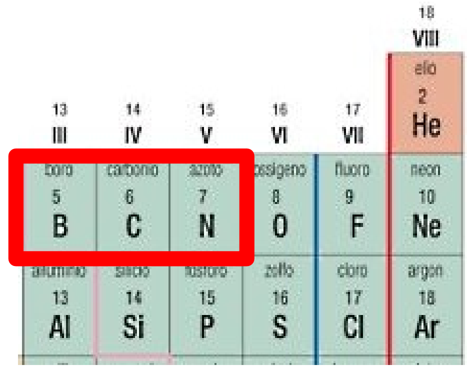
No Gap

Metallic

Graphene vs h-BN

Graphene





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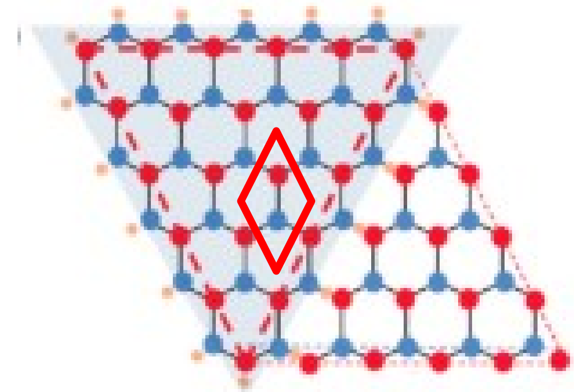
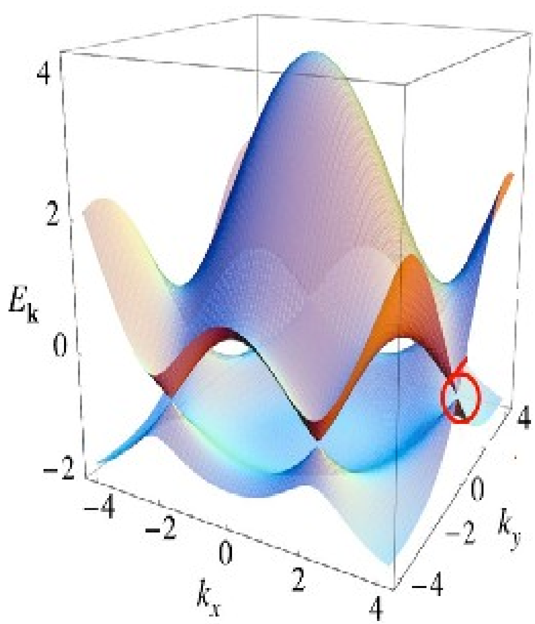


Isoelectronic

Isostructural
2% lattice constant mismatch



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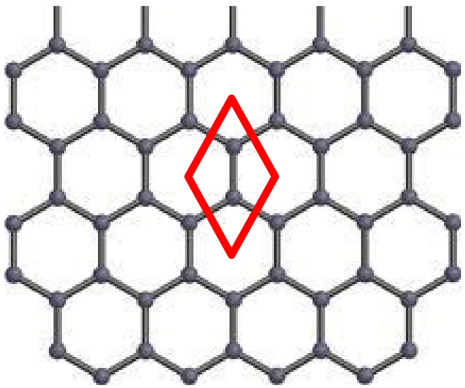

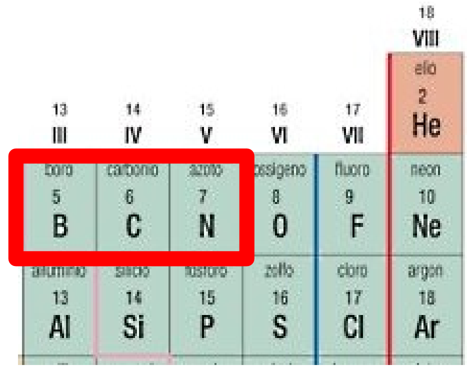

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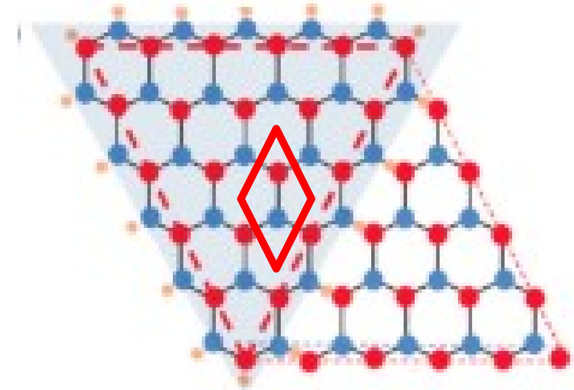

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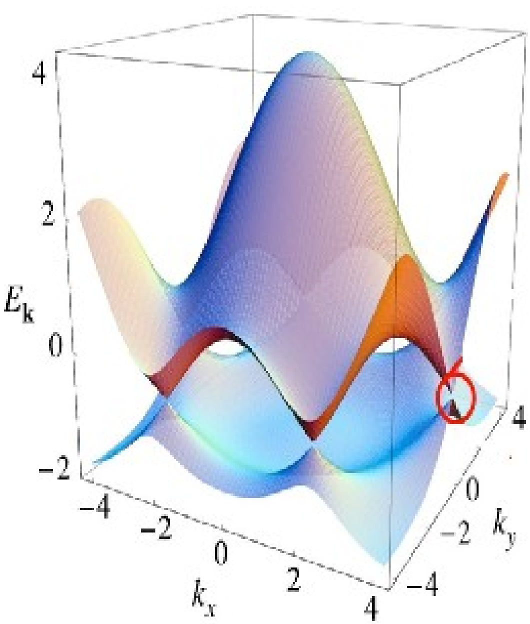
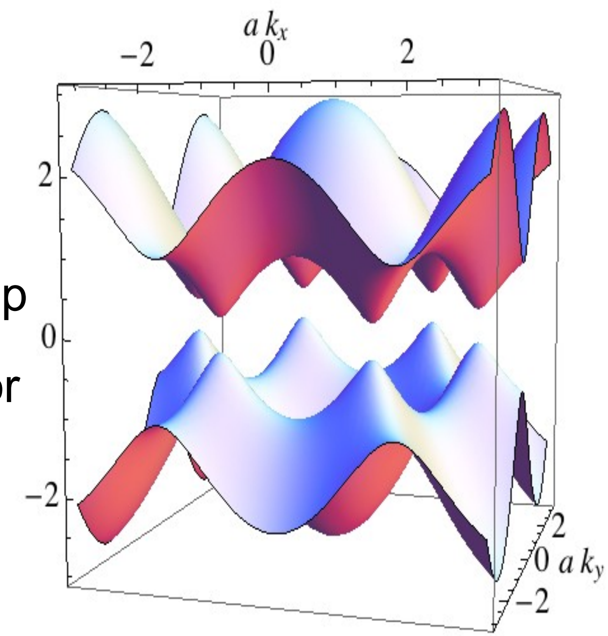


No Gap

Metallic

Bandgap

Insulator



Hybrid BCN systems

Growing of hybrid Gr and h-BN layer

- Hybridized h-$B_xN_xC_y$ structures would have interesting properties combining graphene and h-BN properties

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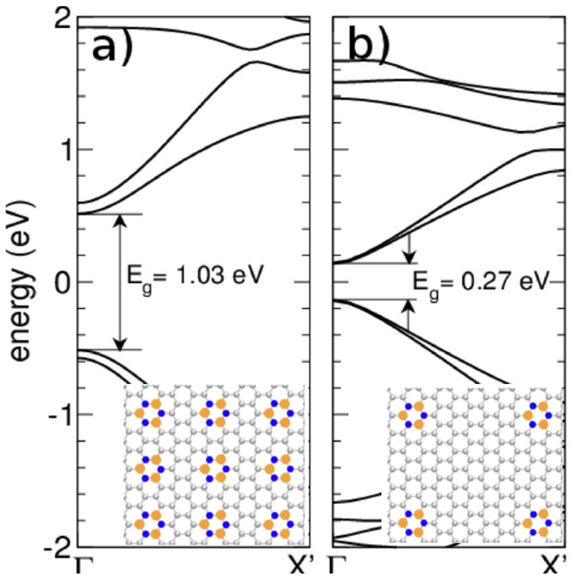
Electronic properties

Radisav S. Krsmanovic et al., J.Phys.Chem.C 118, 16104 (2014)



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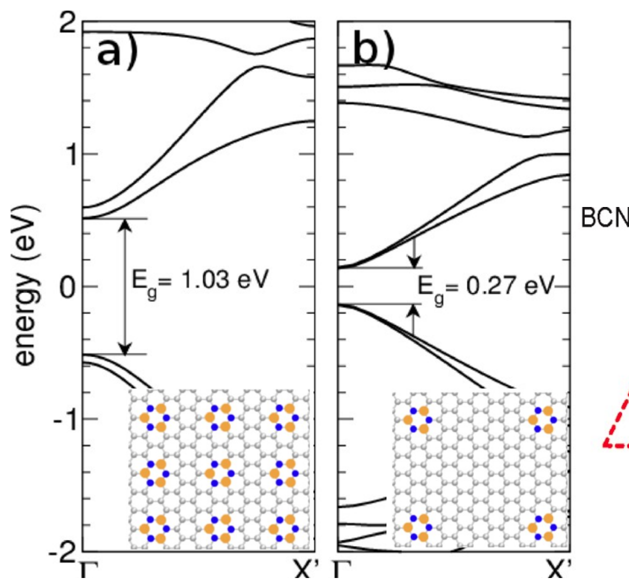
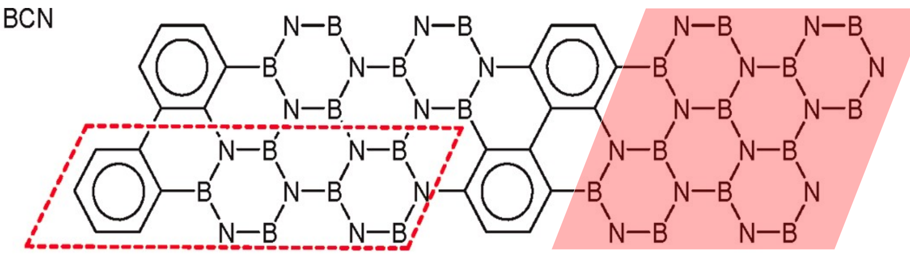


Structural configuration



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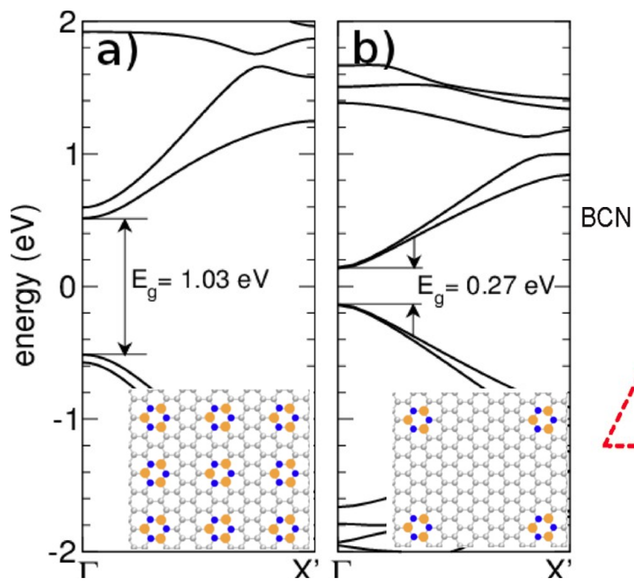

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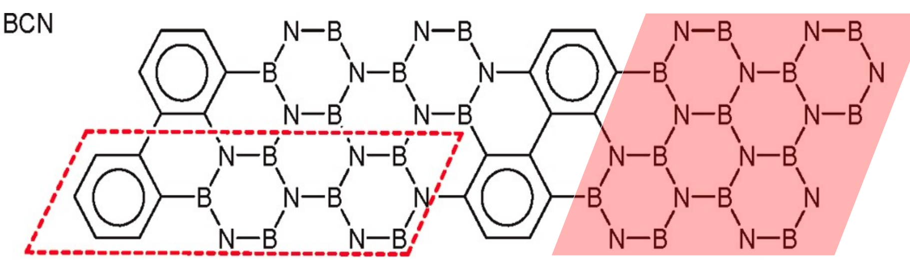

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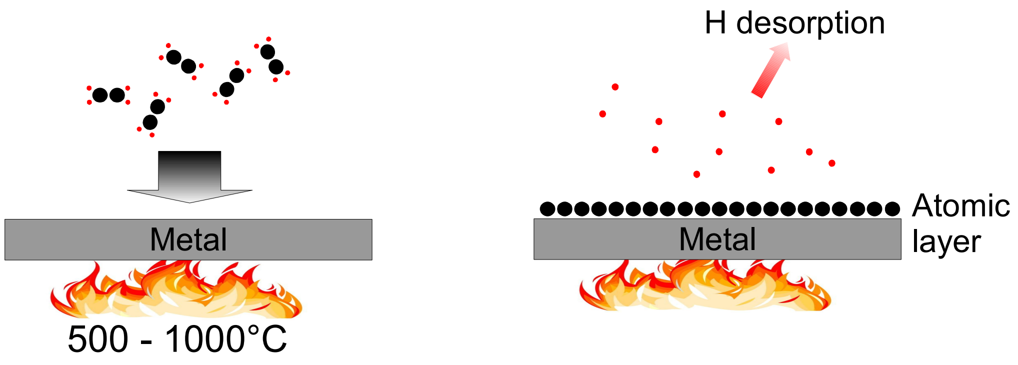
Problems: Phase segregation

"Pure" bonds are preferred to hybrid ones

Zhu.J. et al., J.Phys.Chem.C 115, 10264 (2012)   Lam et al., Appl.Phys.Lett. 98 22101 (2011)

Growth of atomic layer

Epitaxial growth by precursor decomposition on transition metal surfaces



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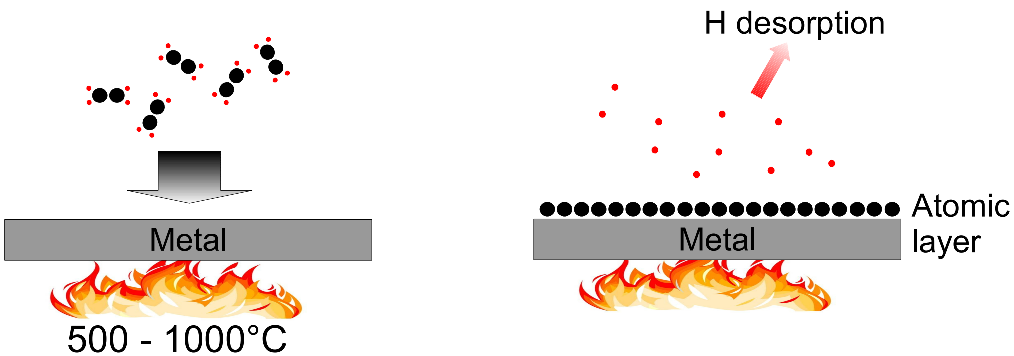

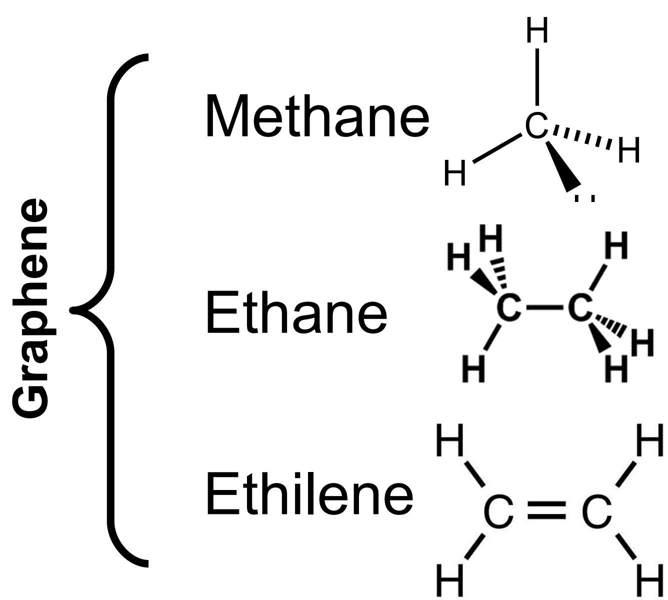

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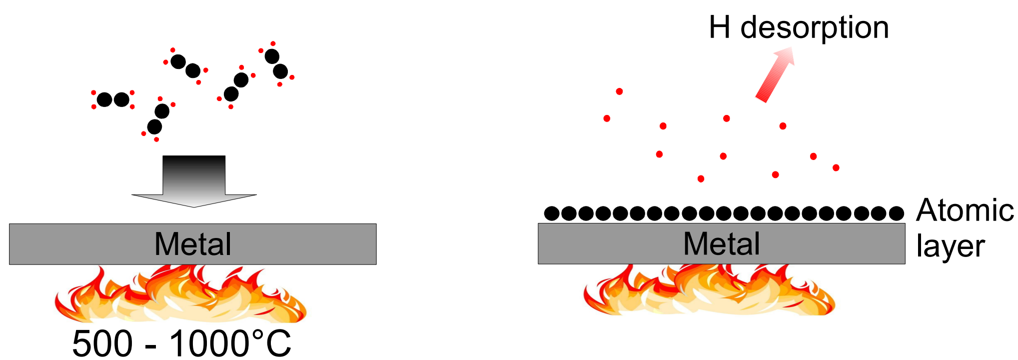
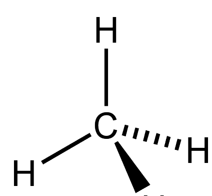
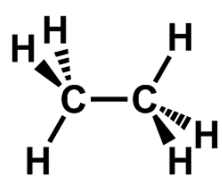


Graphene

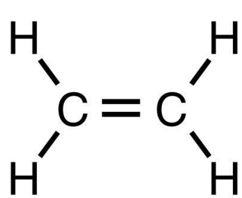
Methane



Ethane



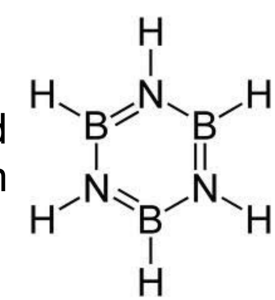
Ethilene



h-BN

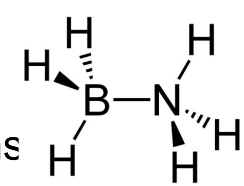
Borazine

Similar to benzene Liquid and not stable at room temperature



Ammonia Borane

Stable at ambient conditions



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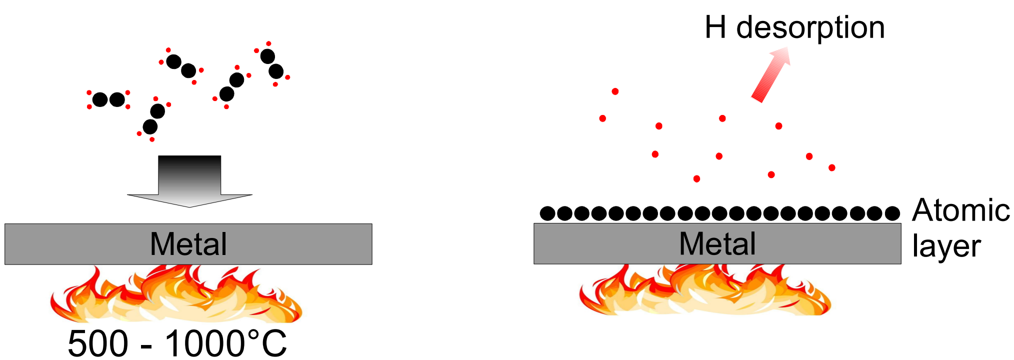
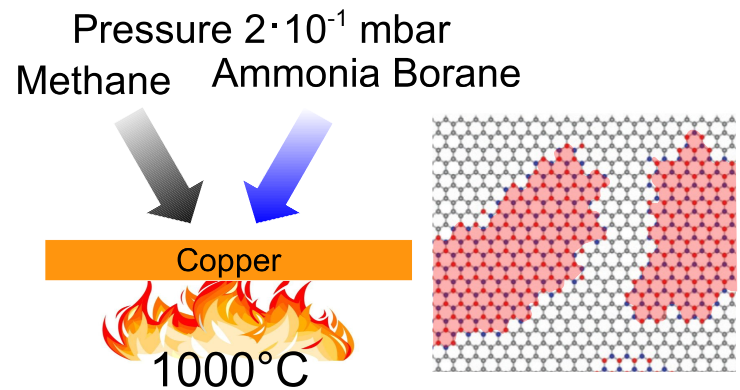
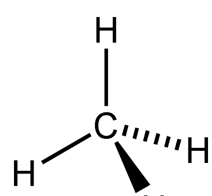




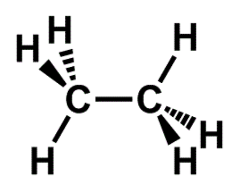
Ci et al. Nature Mat.. **2010**, 9, 430

Graphene

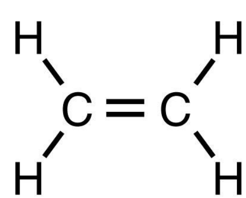
Methane



Ethane



Ethilene



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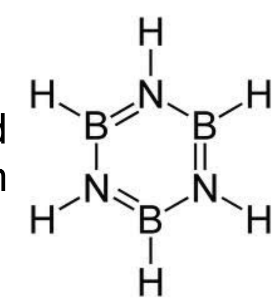

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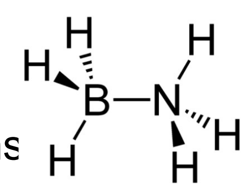
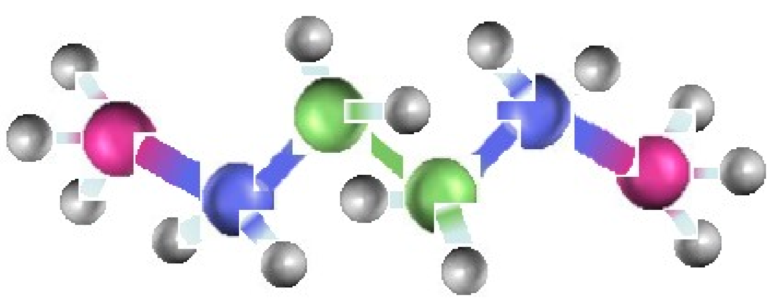


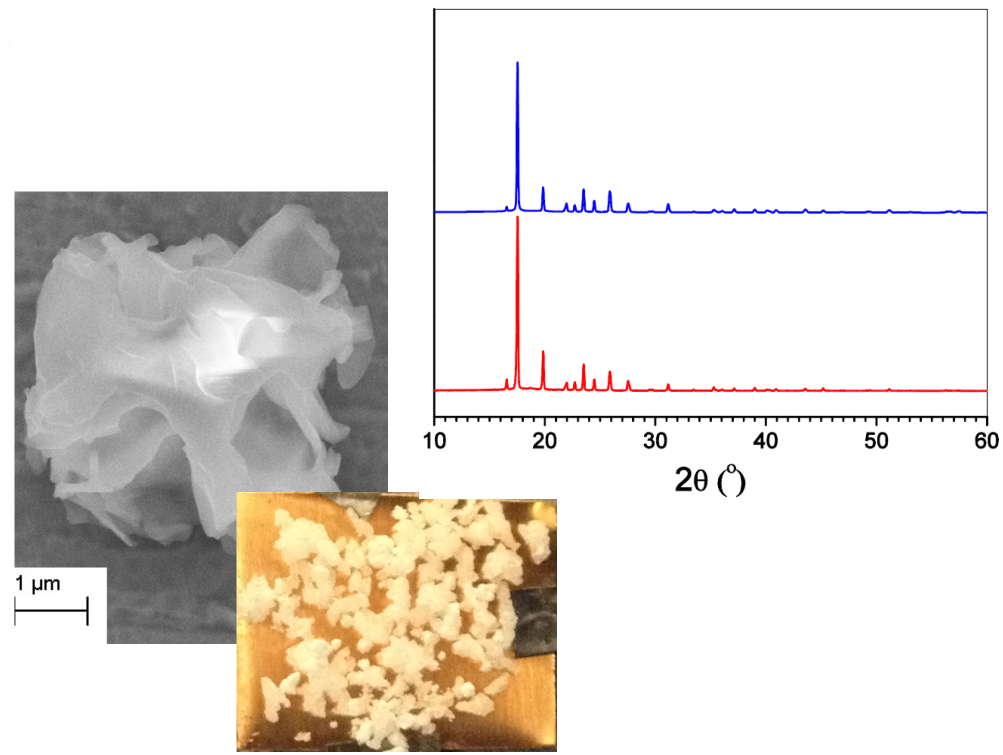
EDAB solid phase characterization

Use a single precursor containing B, C and N atoms instead of two different precursors (one for graphene and one for h-BN)

Ethylenediamine Bisborane
(EDAB)

$BH_3NH_2CH_2CH_2NH_2BH_3$

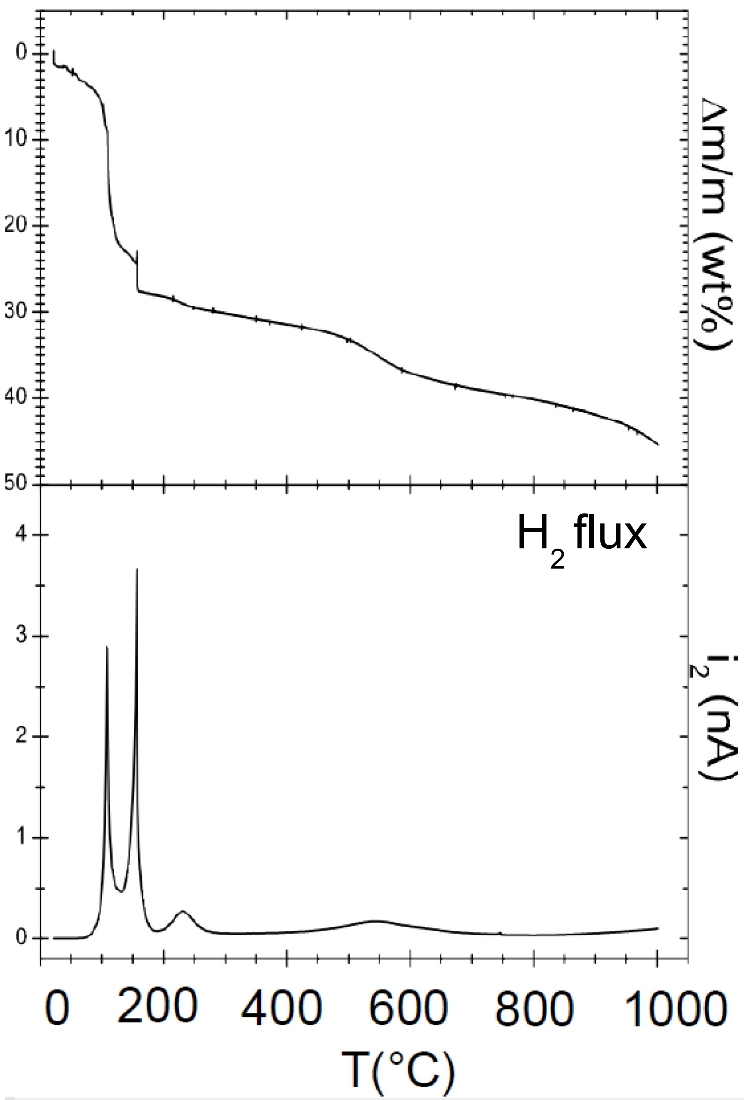




Crystalline at room temperature

EDAB at high temperature

In vacuum thermolysis 10^{-4} mbar



EDAB

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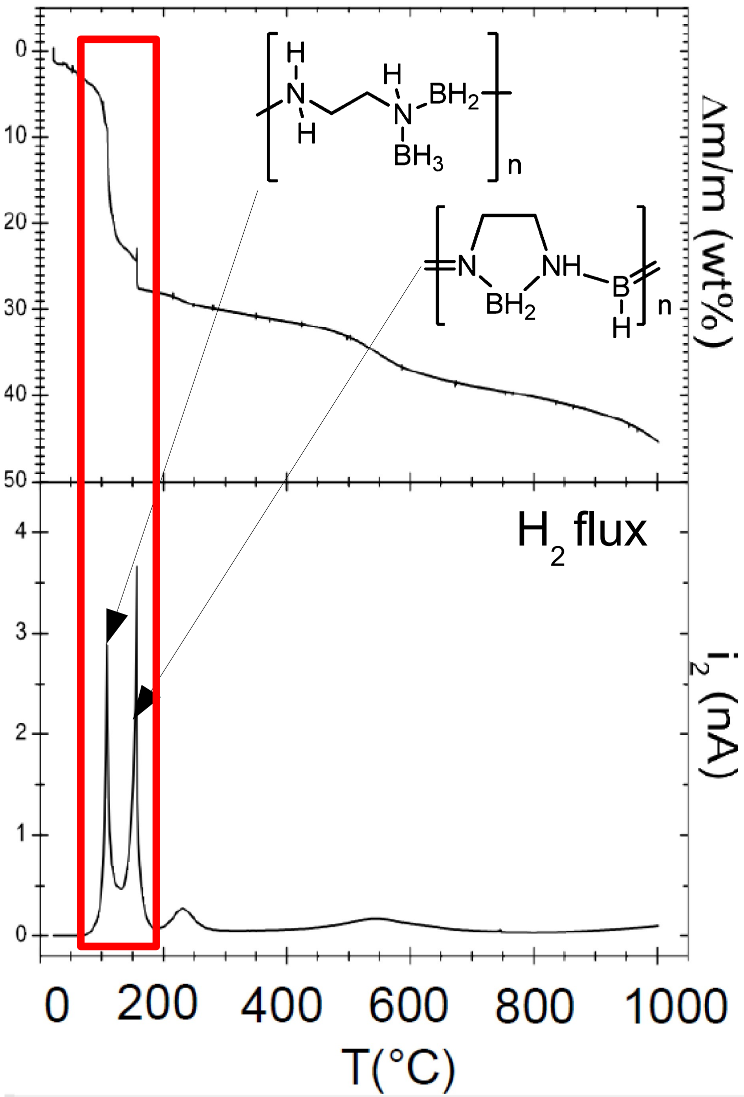
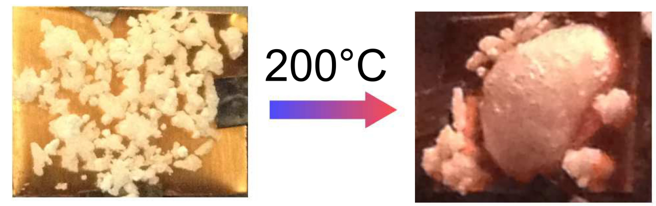


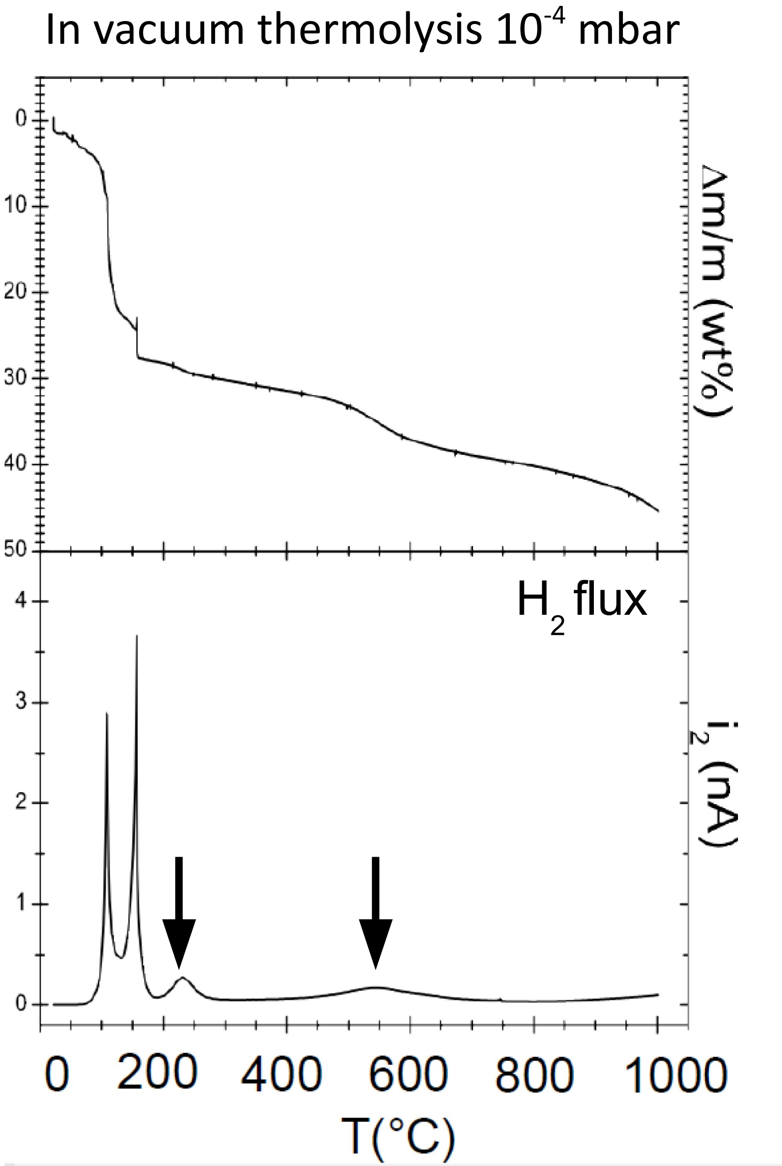


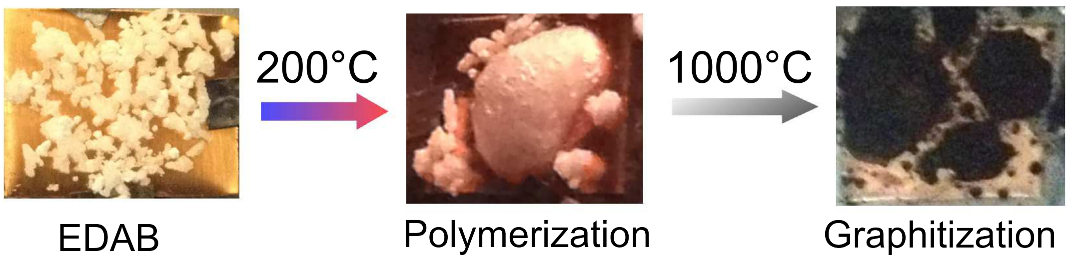
EDAB Polymerization

H_2 desorption events at 108°C, 157°C, and polymerization

Leardini et al. J.Phys.Chem.C **2014**, 118, 17221

EDAB at high temperature





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Desorption peaks at 231°C and 550°C

EDAB at high temperature

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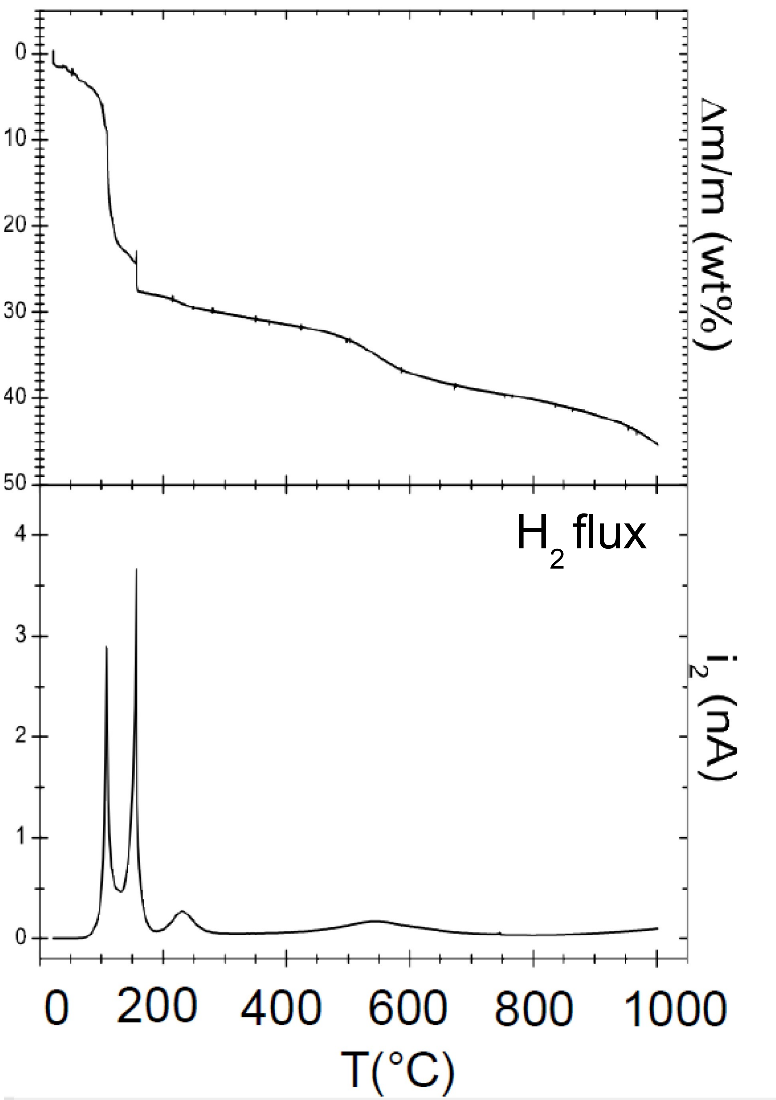

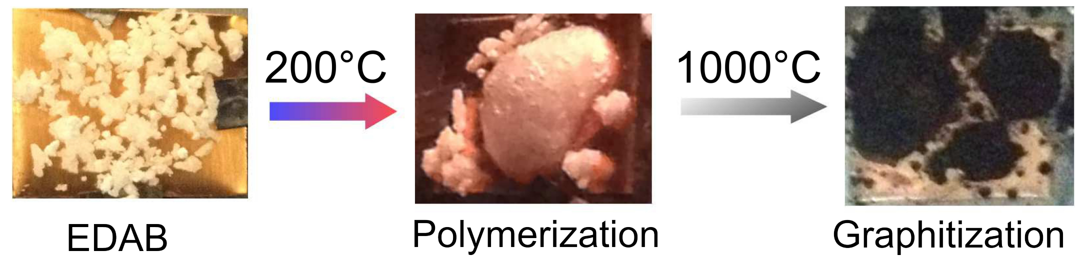

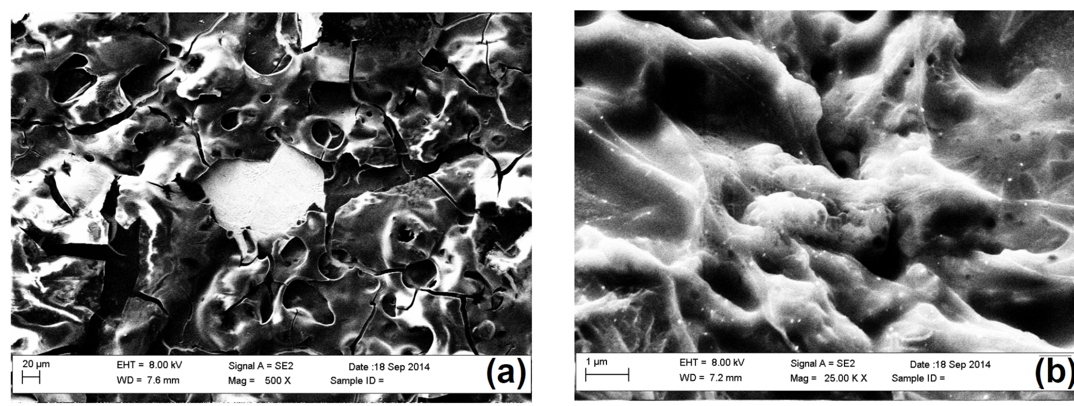

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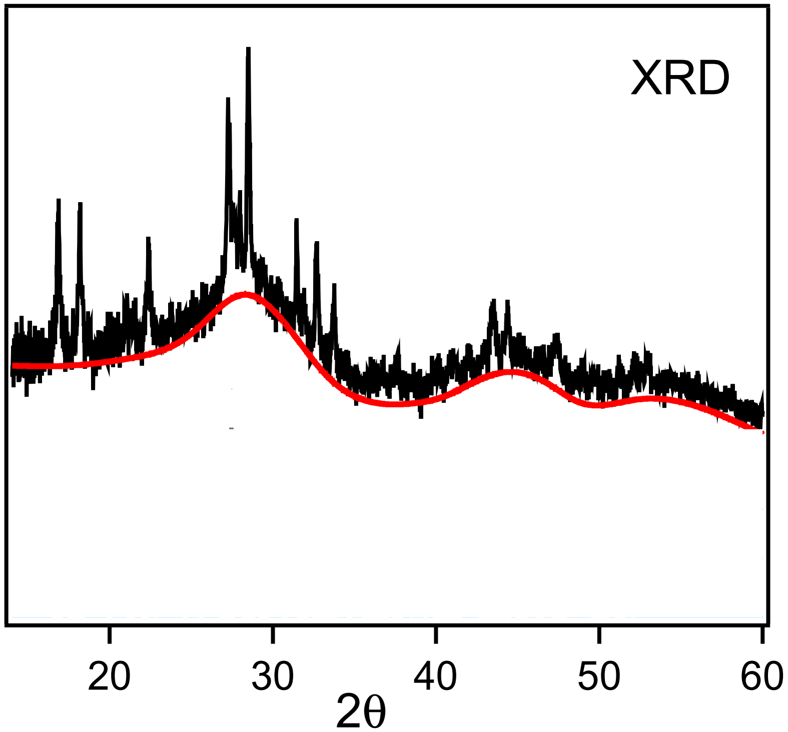
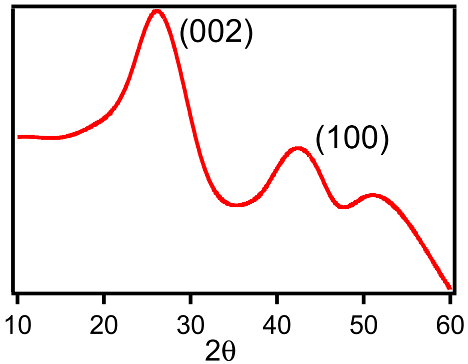
Presence of flake – like regions with sharp edges or compact areas

EDAB at high temperature





XRD broad peaks 2θ = 24.2°, 43.0° of a poorly crystalline graphitic phase

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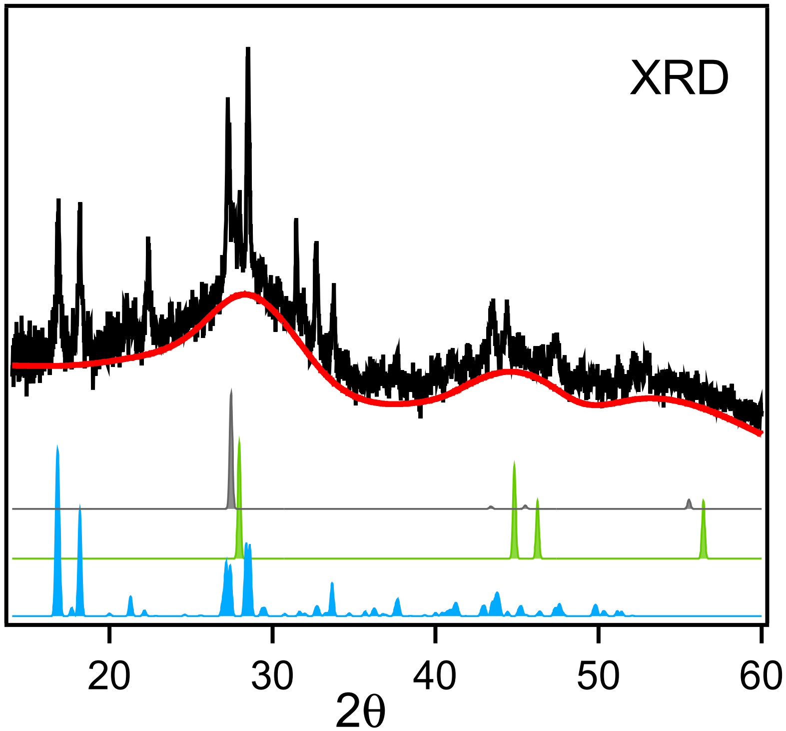

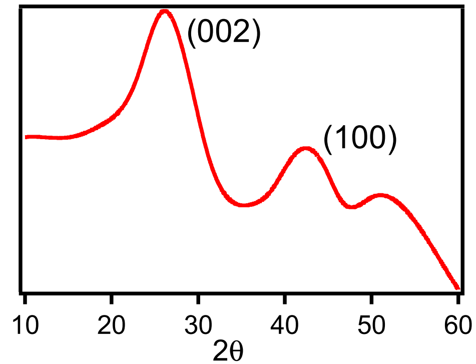

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Sharp diffraction peaks assigned to Ammonium Hydroxide Borate Hydrate (or Ammonium Borate Hydrate $B_5H_{12}NO_{12}$), graphite and $(BN)_{0.26}C_{0.74}$

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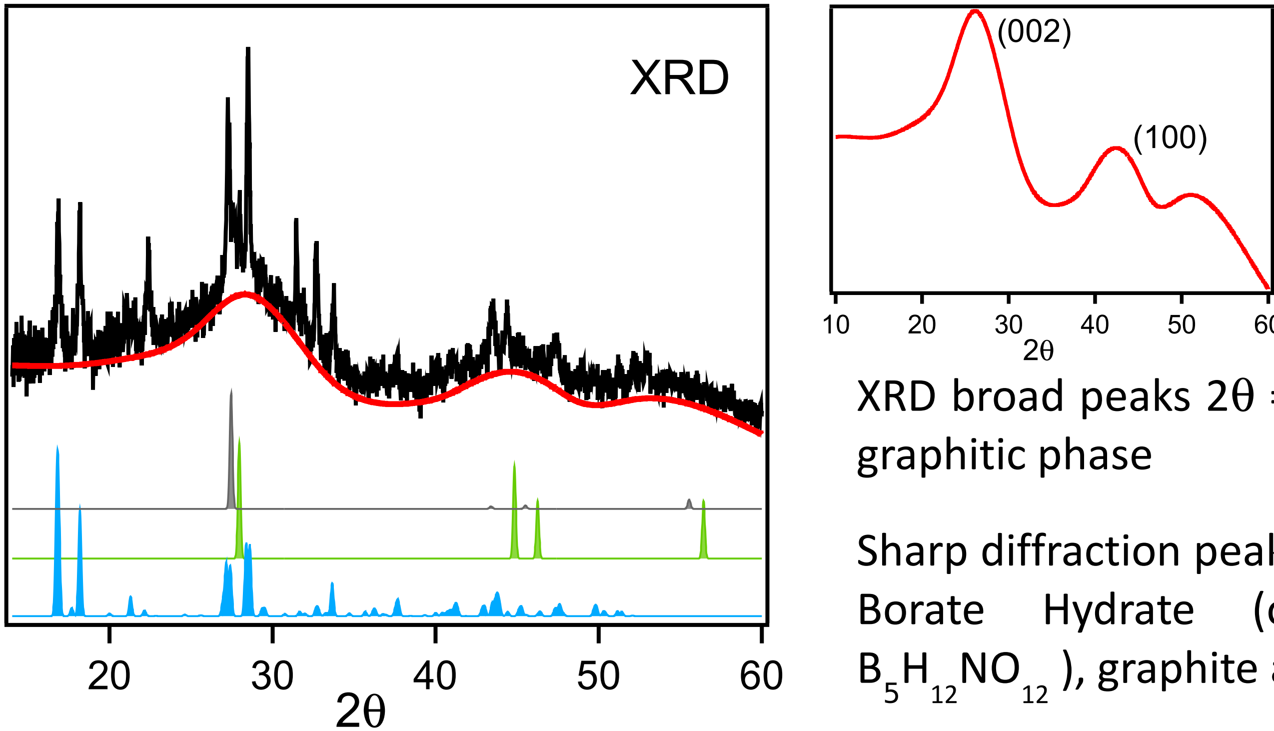

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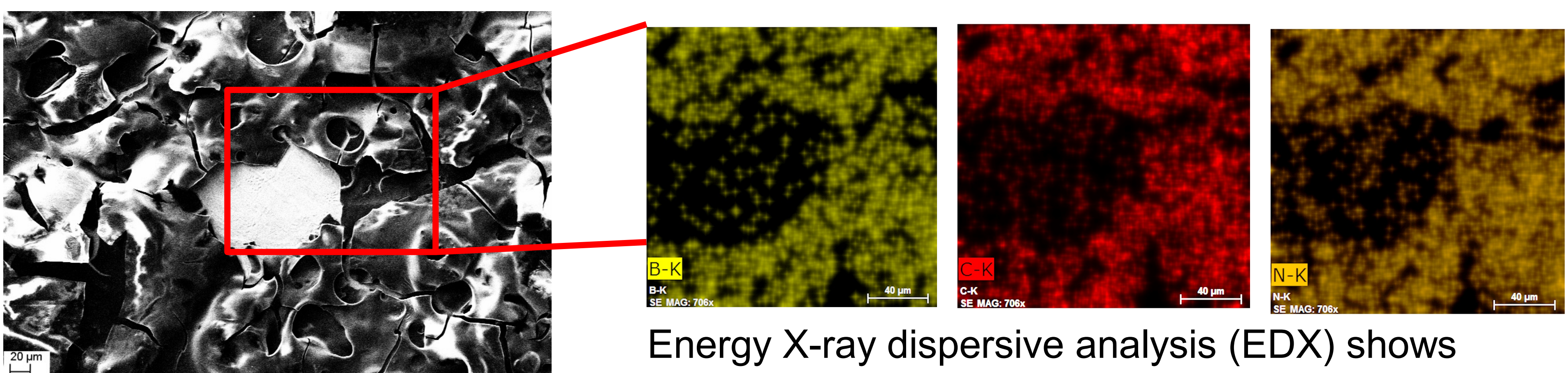
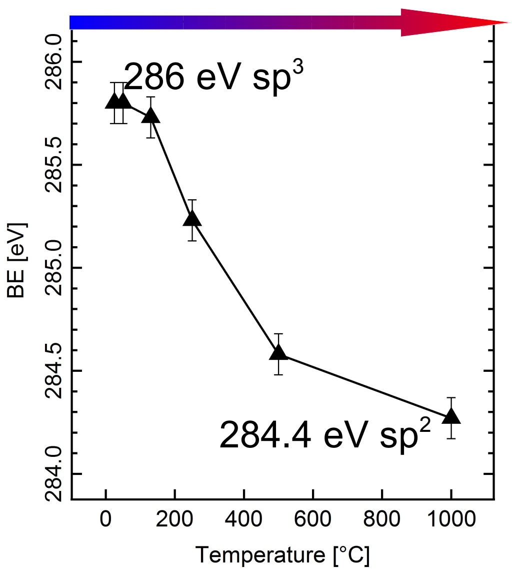


Energy X-ray dispersive analysis (EDX) shows mixing of B, C, N

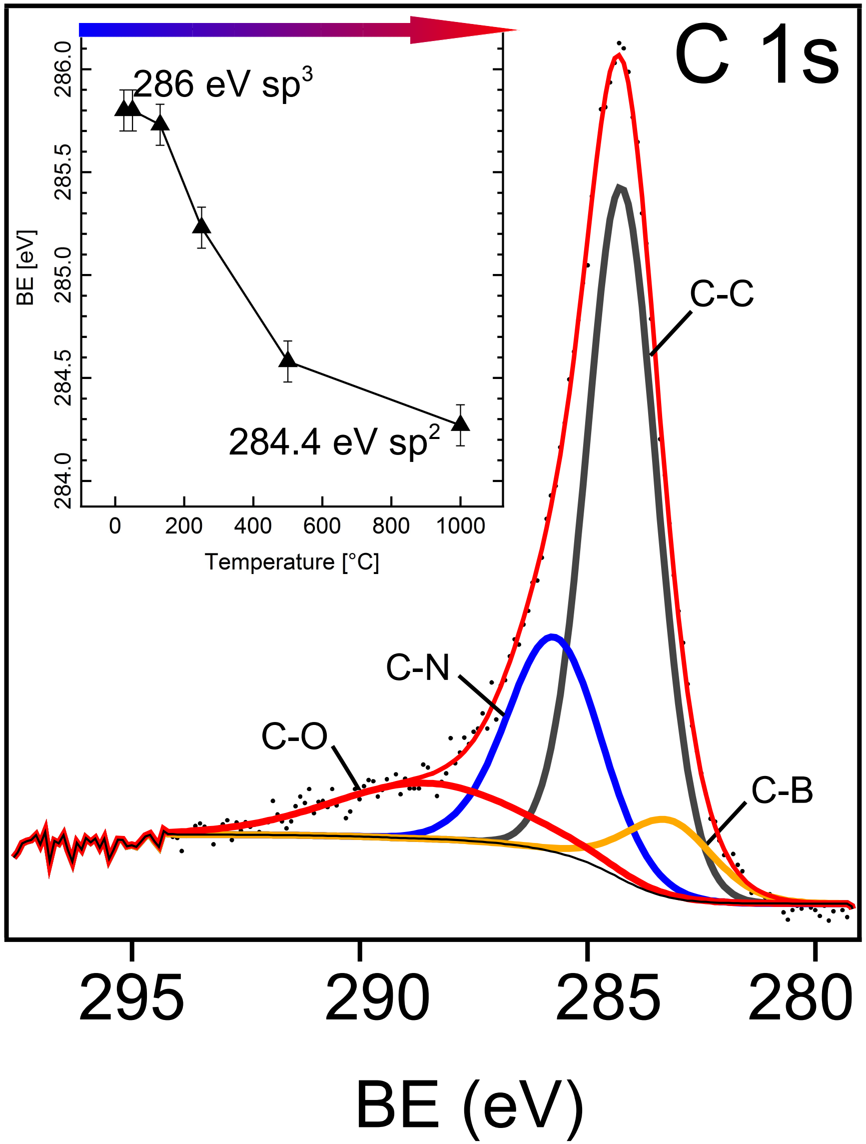
EDAB at high temperature



C 1s from sp3 to sp2 hybridization (284.4 eV)

Wilson et al. Nano Research **2013**, 6, 99

EDAB at high temperature



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Presence of hybrid C – N and C – B bonds

Ci et al. Nature Mat.. **2010**, 9, 430

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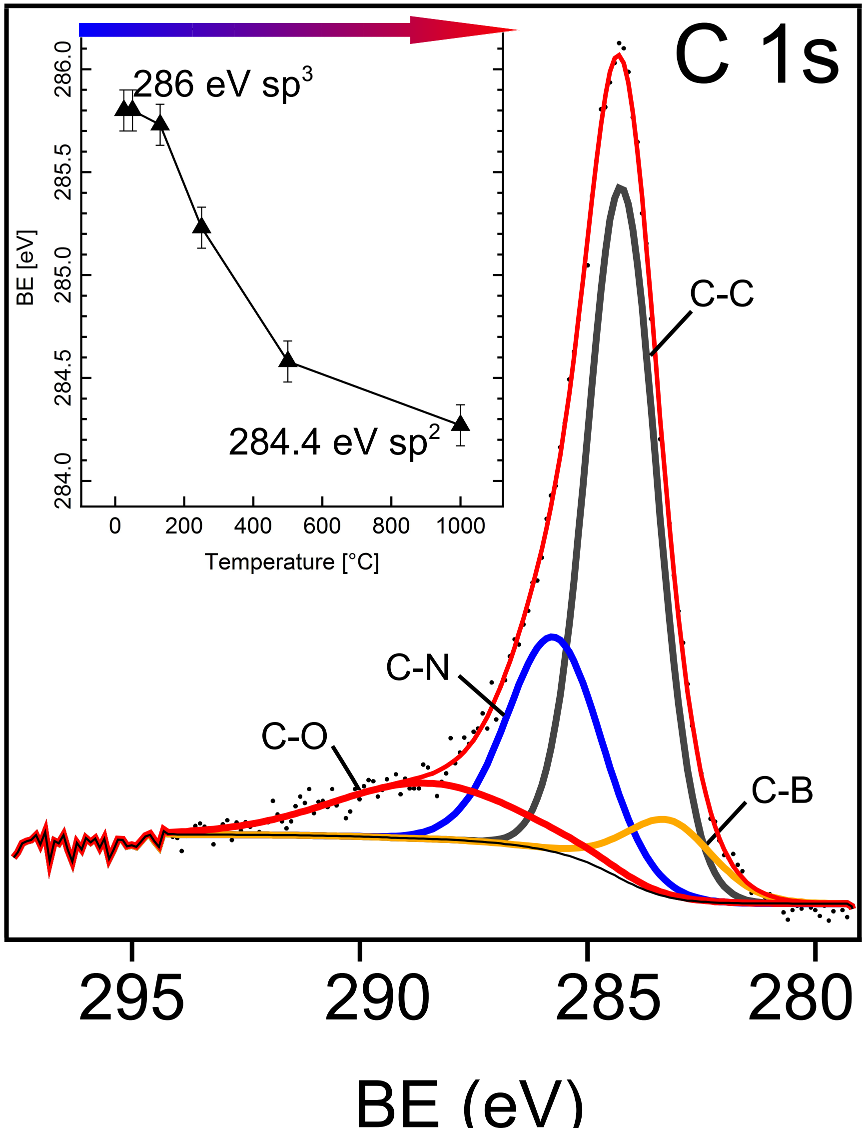

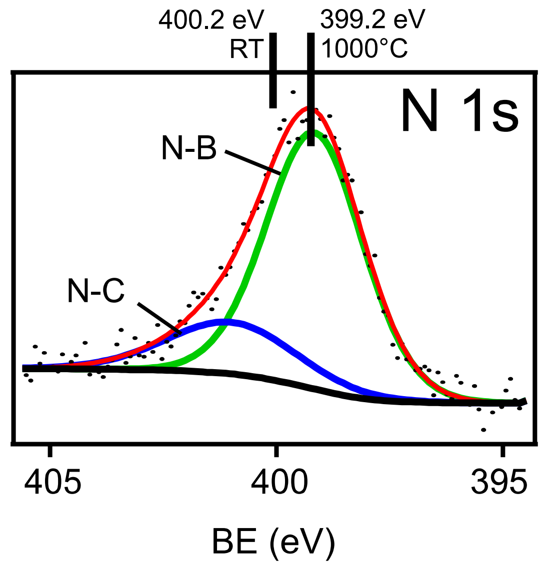

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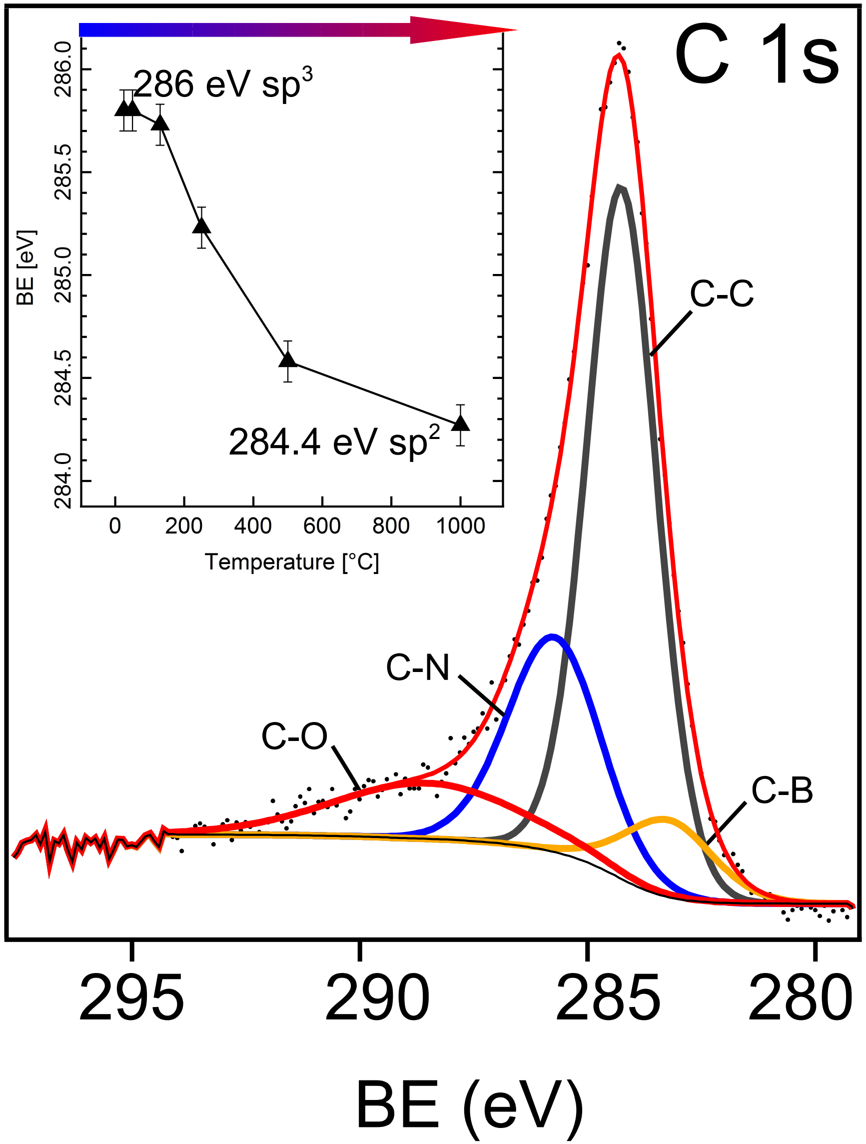

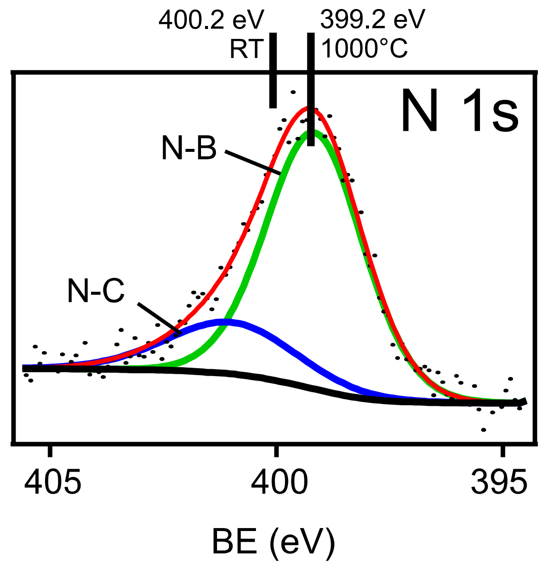

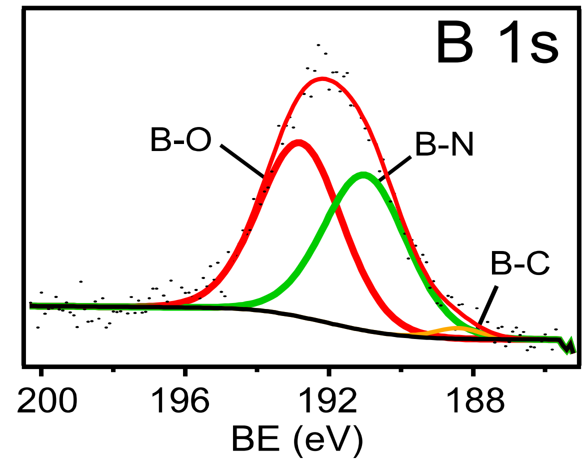

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N 1s (399.2 eV) in agreement with presence of B-N and C-N coordination

B 1s (192.6 eV) in agreement with the presence of prevalent boron oxide mixed with B-N, B-C coordination

B : C : N = 0.2 : 1 : 0.4

Conclusions

Formation of hybrid BCN is a new challenge for scientist providing a new class of monolayer material with tunable electronic structure

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We demonstrate formation of poor crystalline graphitic phase with B and N doping, from high temperature thermolysis of a single molecular precursor (EDAB)

Thank you for your attention