New boron phosphide nanocrystals

Synthesized in molten salt

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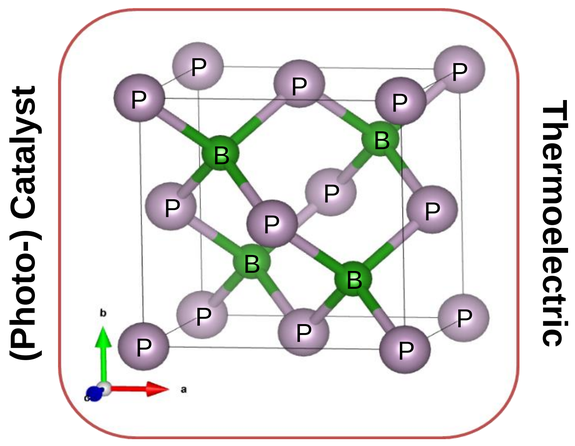
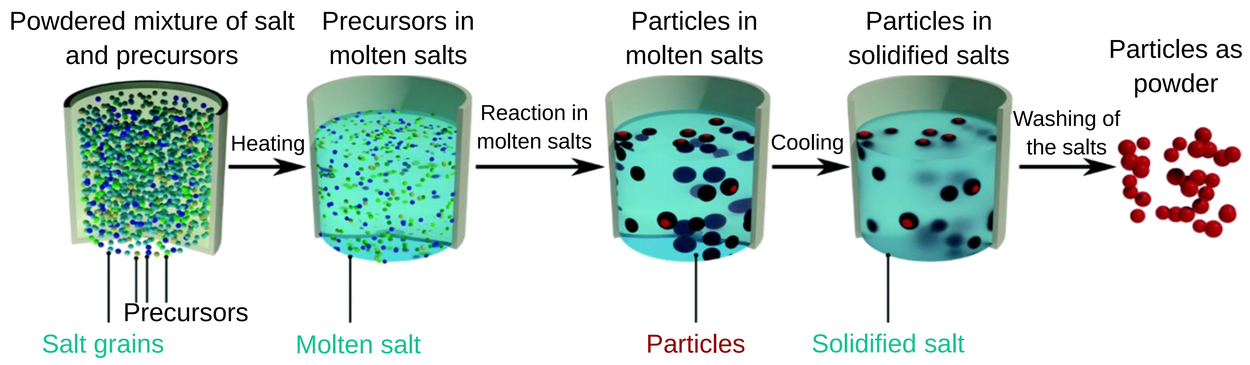
Hard Material



SYNTHESIS

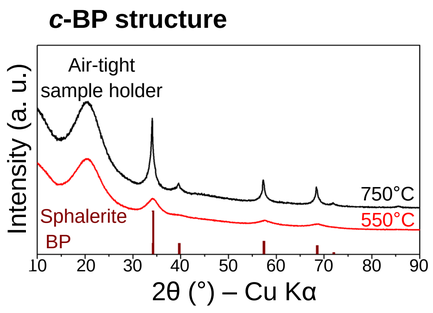
Molten salt synthesis allows the **formation of covalent bonds** and **promotes nanosized objects** [1]



ANALYSIS

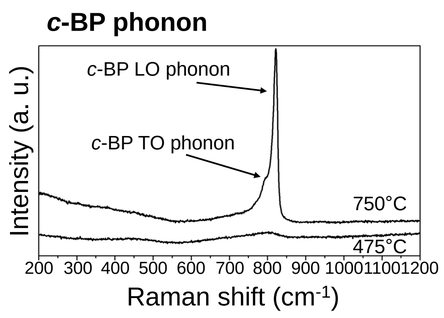
Powder XRD

***c*-BP structure**

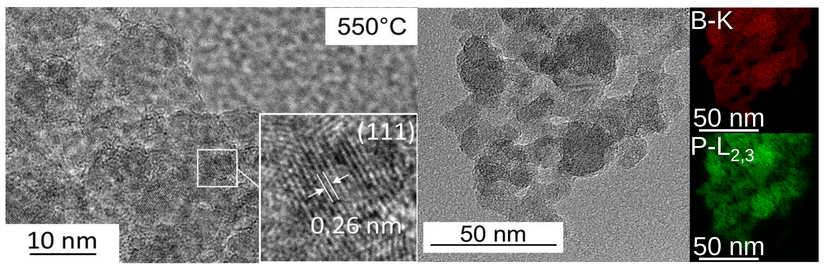


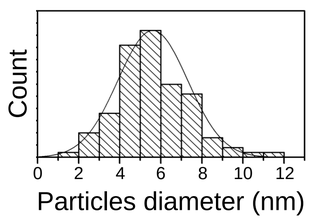
Raman spectroscopy

***c*-BP phonon**



TEM & STEM-EDS

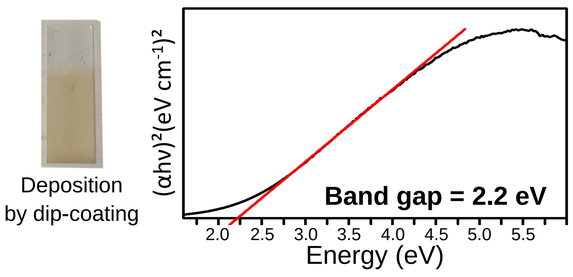


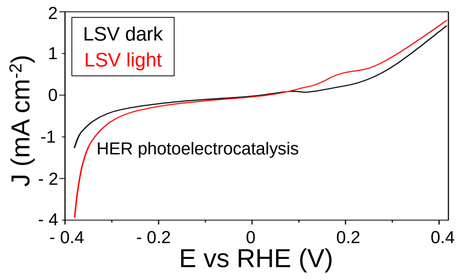


5 nm nanocrystals with **B and P homogeneously distributed**

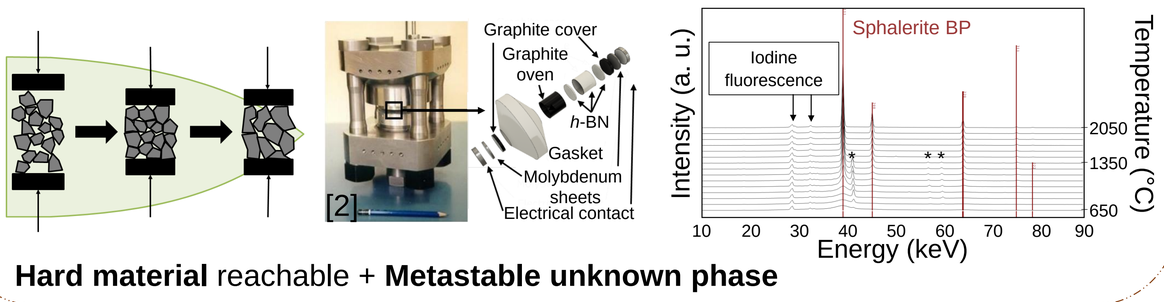
PROPERTIES

Optical and **photoelectrochemical** properties





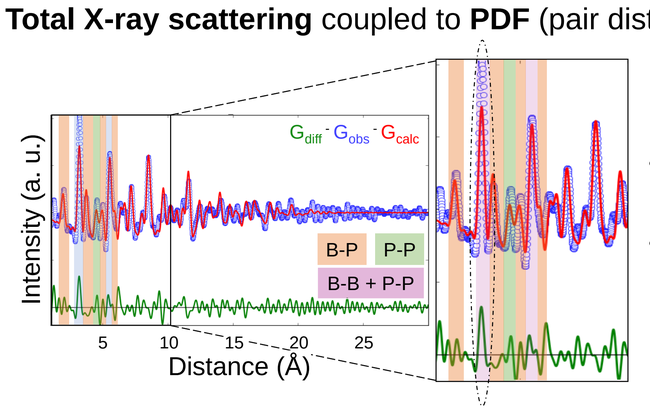
High pressure sintering: ***in operando*** energy dispersive **XRD** – 5 GPa – θ=7°



Hard material reachable + **Metastable unknown phase**

LOCAL ENVIRONMENT

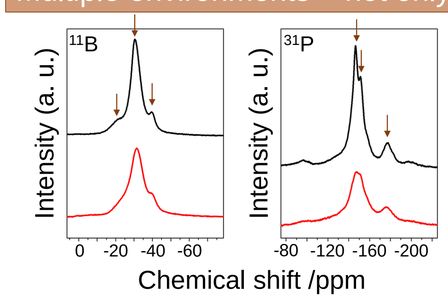
Total X-ray scattering coupled to **PDF** (pair distribution function) analysis



- Strong correlation with *c*-BP pattern
- Lack of contribution at 3.2 Å

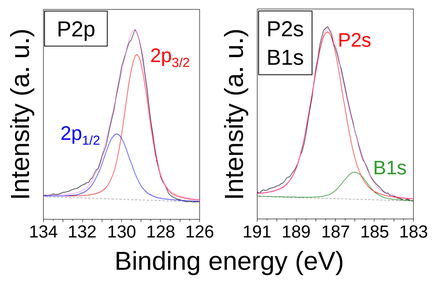
MAS NMR – 700 MHz – 14 KHz – 3.2 mm rotor

Multiple environments = not only Td

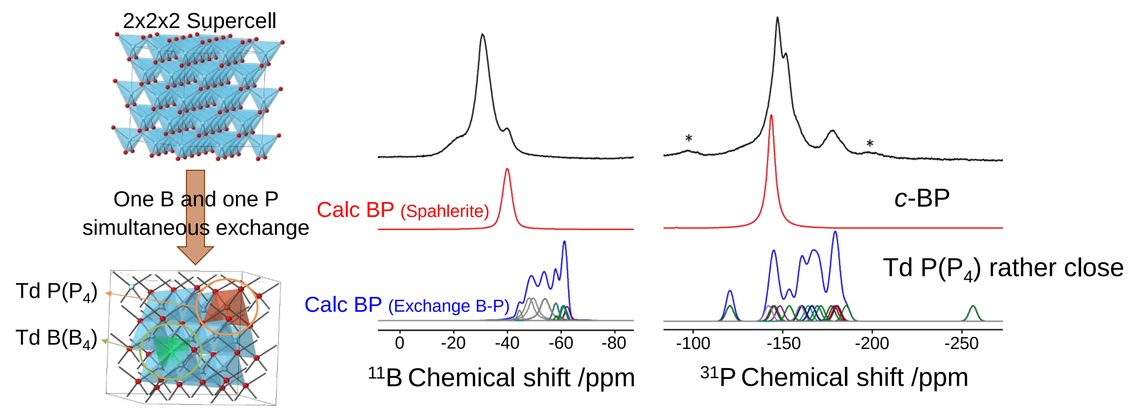


XPS

Elemental P and B at the surface, no oxidation



DFT simulation to identify the multiple environments

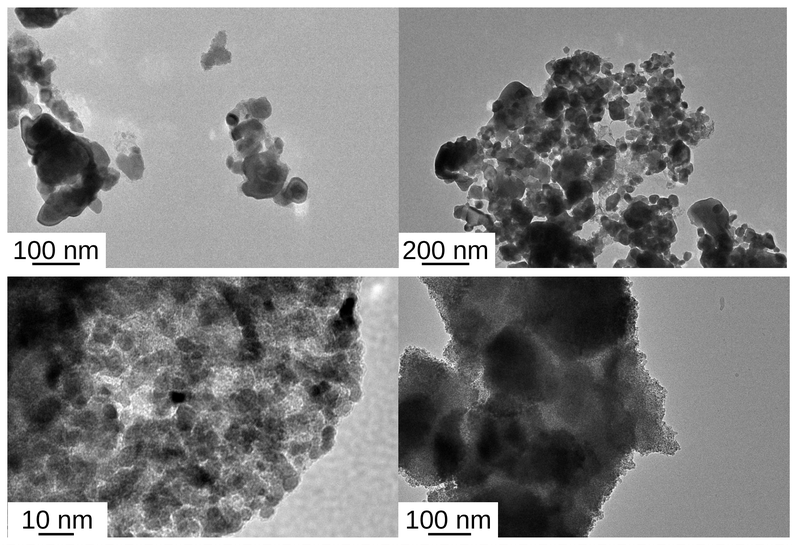


Possible presence of vacancies, ion insertion, and P-rich BP structure.
Simulations under progress

REACTIVITY WITH METALS

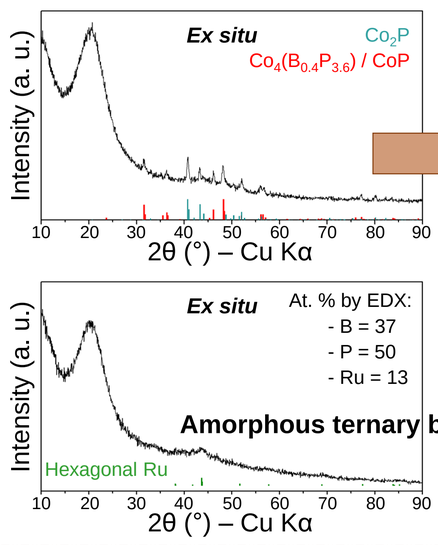
Molten salt synthesis:

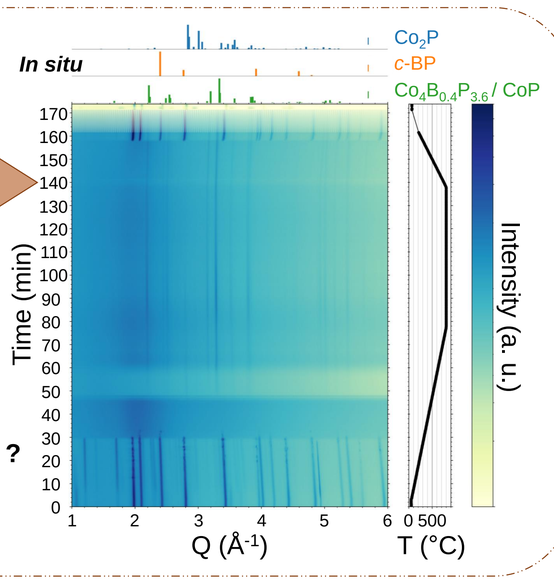
1) *c*-BP + metal salt in molten salt
2) 750°C – 2h
3) Washing
4) Drying (120°C – overnight)



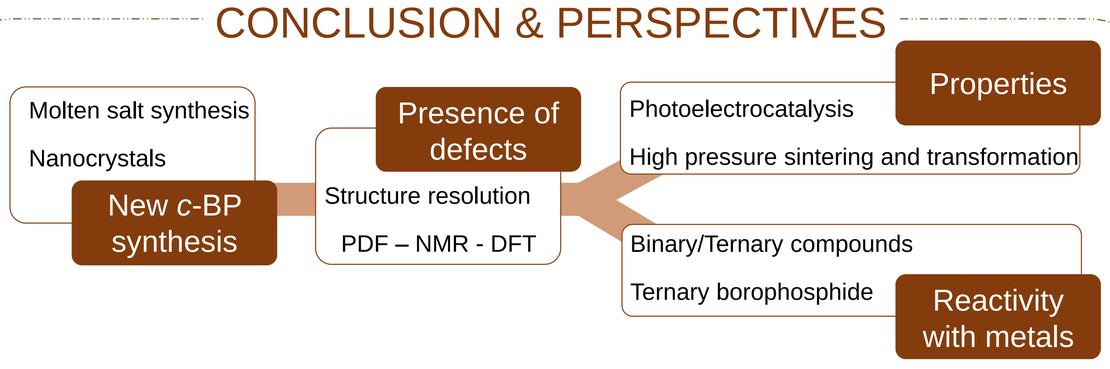
Colloidal synthesis [3]:

1) *c*-BP + $Ru_3(CO)_{12}$ in THF
2) Vigorous stirring - 4h at RT
3) Solvent evaporation
4) Drying - vacuum 6h at 390°C





CONCLUSION & PERSPECTIVES



We developed **a brand new synthesis** to obtain boron phosphide nanocrystals. This material is a **very promising platform to develop functional nanomaterials: high pressure transformations**, **ultra-hardness, photoelectrocatalysis** and their use as reagent to develop **binary and ternary compounds** are among the research tracks currently studied.

REFERENCES

[1] Portehault, D. Gómez-Recio, I. Baron, M. A. Musumeci, V. Aymonier, C. Rouchon, V. Le Godec, Y. *Chem Soc. Rev.* **2022**, *51* (11), 4828-4866
[2] Grosjean, R. Le Godec, Y. Delacroix, S. Gouget, G. Beaunier, P. Ersen, O., Ihiawakrim, D. Kurakevych, O. Chanéac, C. Portehault, D. *Solids. Dalton Trans.* **2018**, *47* (23), 7634-7639
[3] Tang, Y. Kobayashi, Y. Tassel, C. Tamamoto, T. Kageyama, H. *Adv. Energy Mater.* **2018**, *8* (23), 1800800
[4] K. Woo, Lee, K., Kovnir, K. *Mater. Res. Express.* (7) **2016**, *3* (7), 074003

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