Benign-by-design solventless mechanochemical synthesis of 3-, 2- and 1-dimensional hybrid perovskites

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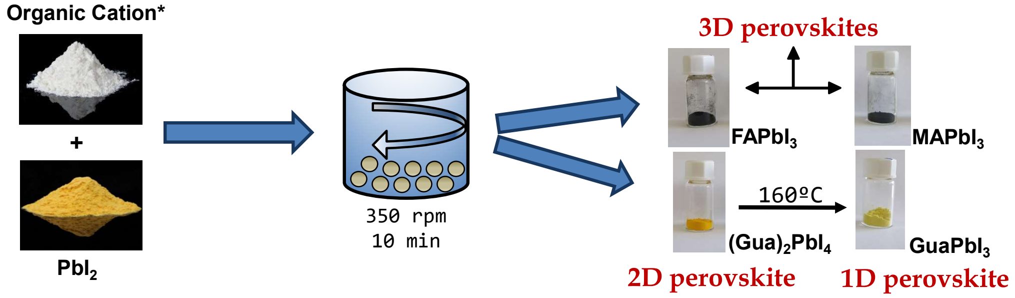
Introduction

Organic-inorganic hybrid perovskites have recently attracted significant attention in the scientific community due to their extraordinary optoelectronic properties with applications in the fields of solar energy, lighting, photodetectors and lasing. The rational design of these hybrid materials is a key factor to optimize their performance in perovskite-based devices. In this work, a mechanochemical approach is proposed as highly efficient, simple and reproducible methodology for the preparation of four types of hybrid perovskites obtaining large amounts of polycrystalline powders with high purity. The synthesis of two archetypal three-dimensional (3D) perovskites ($MAPbI_3$ and $FAIPbI_3$) was accomplished, together with a bidimensional (2D) perovskite $(Gua)_2PbI_4$) and a "double-chain" perovskite ($GuaPbI_3$), whose structure has been elucidated for the first time by using X-ray diffraction.

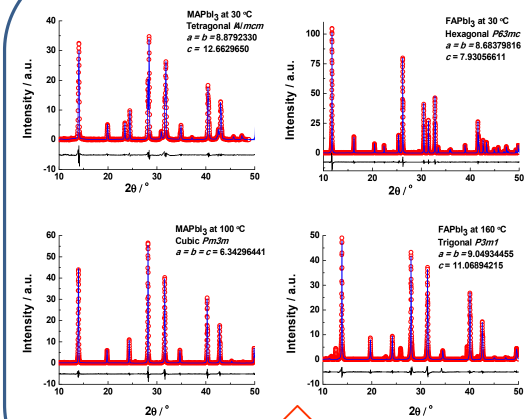
Mechanosynthesis of hybrid Perovskite



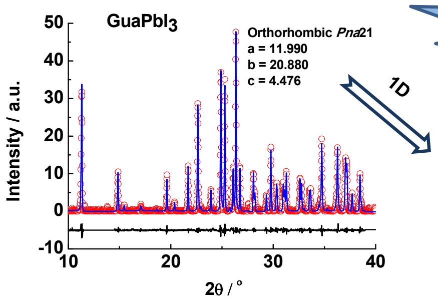
- **Simple**
- **Faster**
- **Reproducible**
- **Highly efficient**
- **Solventless**

*Metilammonium Iodide (MAI) , Formamidinium Iodide (FAI) and Guanidinium Iodide (GuaI)

X-ray Structural studies

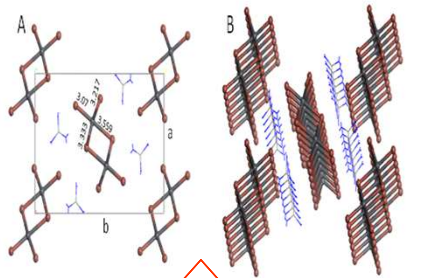


Pawley fits of the XRD patterns with very good agreement with the simulated ones ⟶ Crystallinity and no impurities or precursors



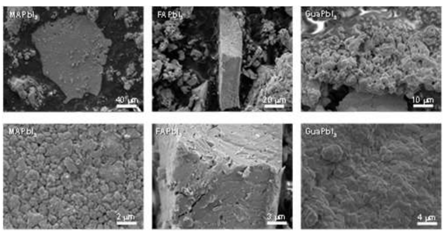
An excellent agreement could be observed between both patterns with no residual reflection peaks from any other concurrent structure.

NEW PEROVSKITE WAS BORN!!!



Crystal structure of $GuaPbI_3$.
1D perovskite

Scanning Electron Microscopy

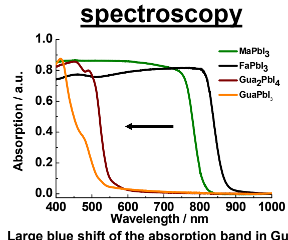


Large size of synthesized crystals.

↓

Positive effect on potential applications of these materials.

UV-vis diffuse-reflectance spectroscopy



Large blue shift of the absorption band in $GuaPbI_3$

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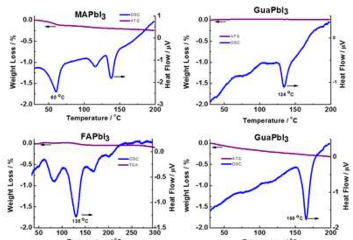
Associated to the disruption of the 3D network of PbI_6^- octaedra

Thermal analysis



No significant weight loss. ⟶ Good stability.

Conclusion

In conclusion, the proposed mechanochemical synthesis offers a simple, efficient and highly reproducible approach for the design of advanced hybrid perovskites, including 3D, 2D and 1D materials. This solventless synthetic method is expected to pave the way for further discoveries and design of novel perovskite materials with innovative properties. Additionally, the facile and cost-efficient preparation of large quantities of the perovskite materials (ca. 5-10 g per batch) remarkably simplifies their use in unexplored strategies for optoelectronics applications.

Acknowledgements

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