Luminescence mechanism of lead-free double perovskite Cs2NaBiCl6 crystal under high pressure

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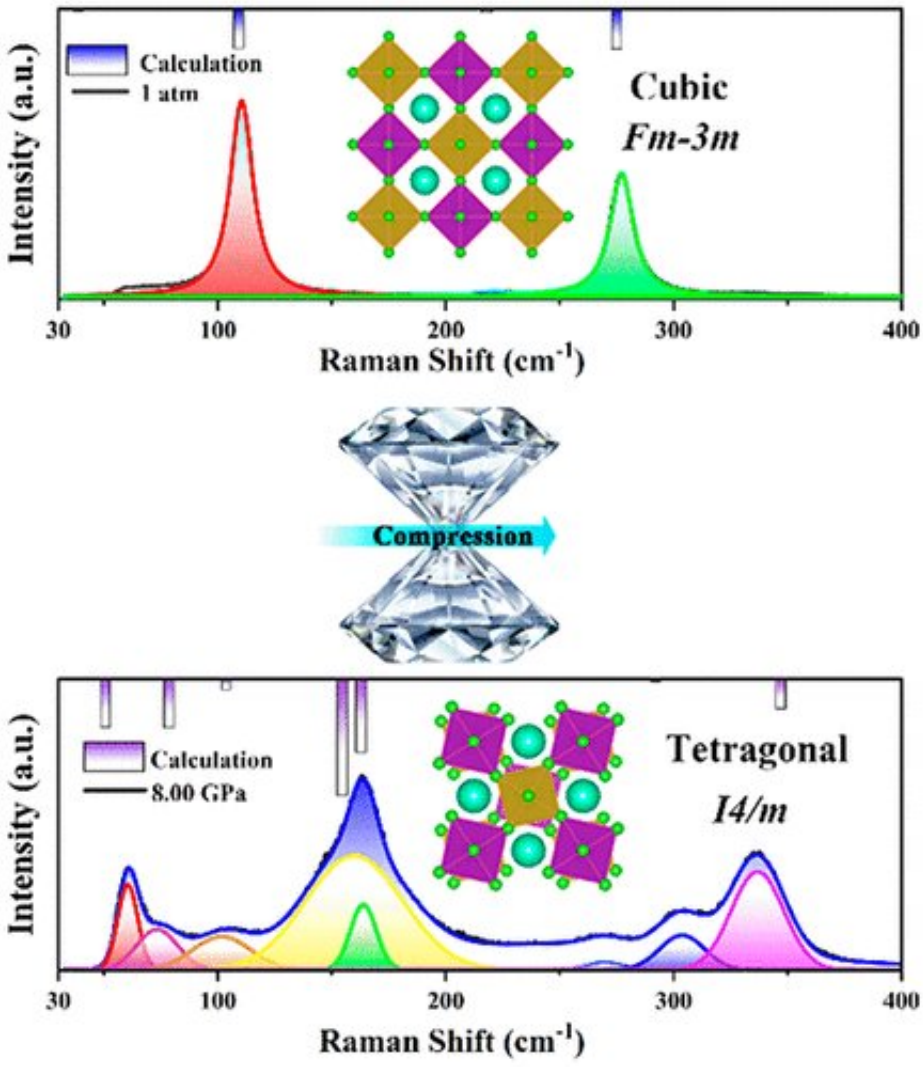

Graphical abstract. Credit: DOI: 10.1021/acs.jpclett.1c02072

High pressure, as an extreme condition, can effectively change the interaction between atoms inside a material, forcing the electronic structure and optical properties to change. Studying the optical and ultrafast dynamical properties of materials under pressure is helpful to understand the relationship between the structure and properties of materials.

Recently, Prof. Yuan Kaijun's group from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS) revealed the luminescence mechanism of $Cs_2NaBiCl_6$ crystal under high pressure by using a comprehensive steady-state and transient spectral characterization system.

This study was published in *Journal of Physical Chemistry Letters* on July 28.

The researchers found that the non-luminous cubic phase $Cs_2NaBiCl_6$ transformed into tetragonal phase at high pressure, which resulted in the distortion of $[BiCl_6]^{3-}$ octahedron and produced dual-color emission self-trapped exciton fluorescence.

By analyzing the results of in situ high-pressure experiments and the density functional theory, they revealed that the dual-color emission was attributed to singlet self-trapped excitons (STEs) and triplet STEs, respectively.

Moreover, they observed the transformation of dark and bright excitons in $Cs_2NaBiCl_6$ crystal by femtosecond transient absorption experiments at different pressures.

"This work provides a deep understanding about the relationship between the self-trapped exciton emission and the crystal structure under pressure. It may offer a guidance for designing and preparing new lead-

free double perovskites," said Prof. Yuan.

More information: Jutao Jiang et al, Transformation between the Dark and Bright Self-Trapped Excitons in Lead-Free Double-Perovskite Cs2NaBiCl6 under Pressure, *The Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/acs.jpclett.1c02072

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