High-pressure study of double perovskite $Cs_2Na_{0.6}Ag_{0.4}InCl_6$: Bi^{3+}

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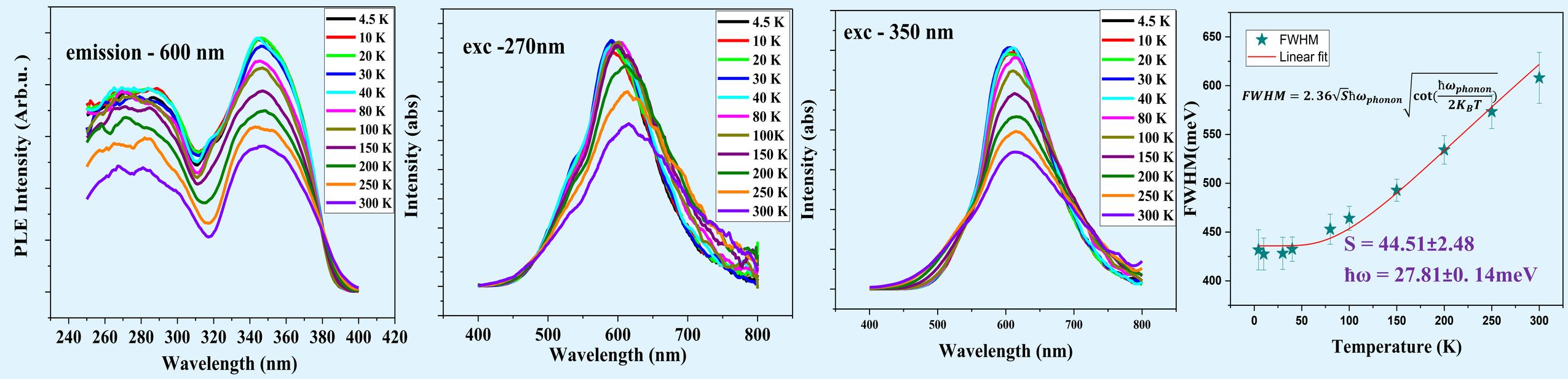
Diamond Anvil Cell cryoDAC-LT (Almax easyLab)

Motivation and aim of the work

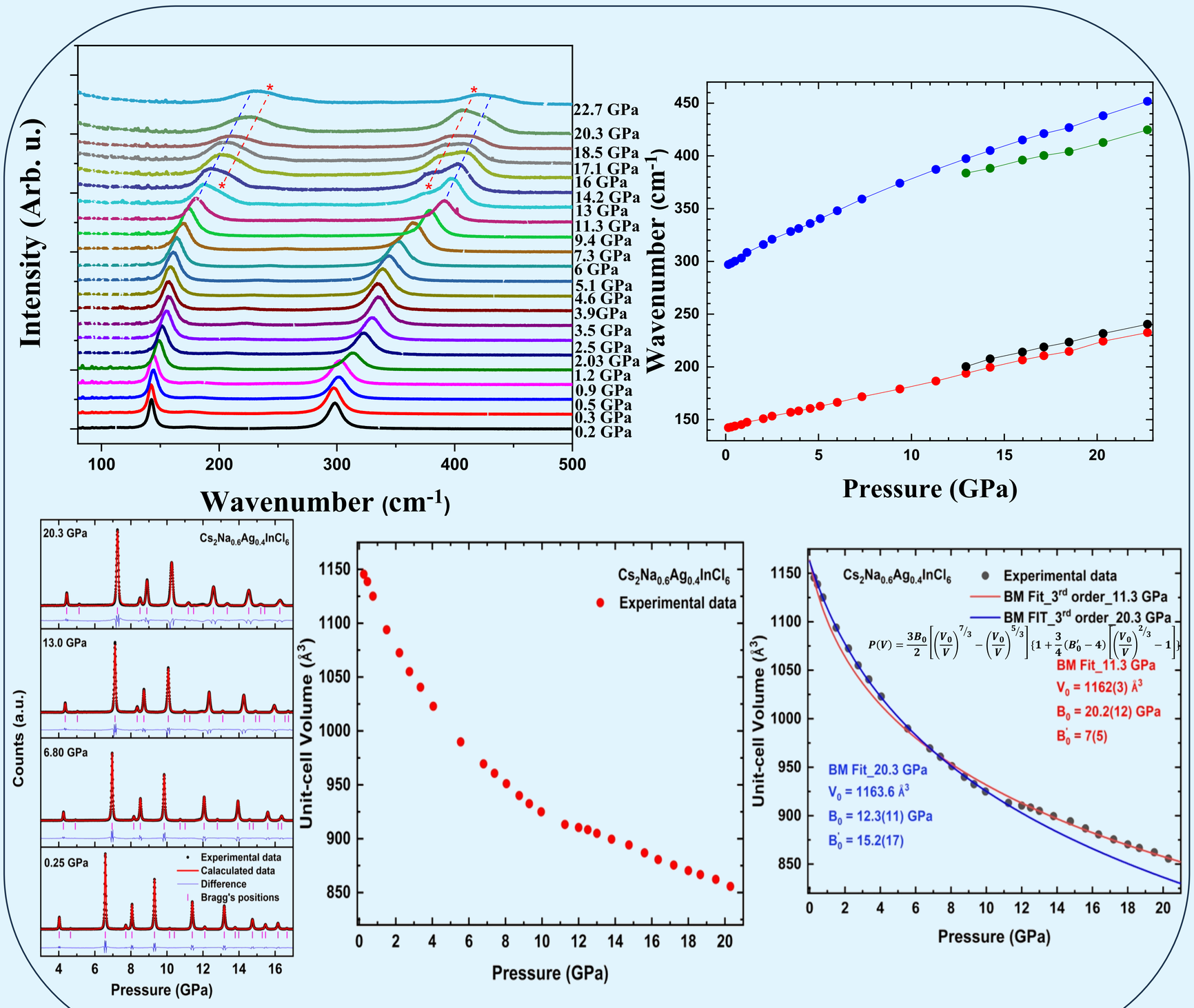
- **Toxicity is a major threat to perovskites' expansion into the field of applications.**
- **Development of lead-free perovskites with desirable characteristics.**
- **$A_2B(I)B(III)X_6$ structured lead-free halide double perovskites (LFHDPs) have gained attention as stable, environmentally friendly alternatives to conventional ABX_3 lead-based perovskites.**
- **Elucidate optical properties of $Cs_2Na_{0.6}Ag_{0.4}InCl_6$:$Bi^{3+}$ double perovskites.**
- **Investigate phase transitions of $Cs_2Na_{0.6}Ag_{0.4}InCl_6$:$Bi^{3+}$ double perovskites.**

Temperature-dependent luminescence studies



Temperature-dependent PLE&PL spectra

High-pressure measurement studies



High-pressure Raman spectra & XRD pattern

SUMMARY

- **$Cs_2Na_{0.6}Ag_{0.4}InCl_6$: Bi^{3+} exhibiting warm white light broad emission spectrum (400-800 nm) attributed to self-trapped excitons caused by a distortion of $AgCl_6$ octahedra due to Jahn Teller effect.**
- **The highest-frequency mode at 296.9 cm^{-1} can be assigned to the symmetric stretching A_{1g} vibration of $InCl_6$ octahedra.**
- **The mode at 142.2 cm^{-1} can be assigned the asymmetric stretching E_g vibration of $InCl_6$ octahedra.**
- **High-pressure XRD and Raman spectroscopy reveal a phase transition of this compound ~11 GPa from cubic to tetragonal I4/mmm structure.**

References

1. **The Journal of Physical Chemistry Letters 11.22 (2020): 9572-9578.**
2. ***Small* 16.31 (2020): 2002547**
3. ***Advanced Functional Materials* 34.13 (2024): 2312316**

Acknowledgments

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