Temperature-dependent studies of 2D-layered perovskite $ThMA_2PbI_4$

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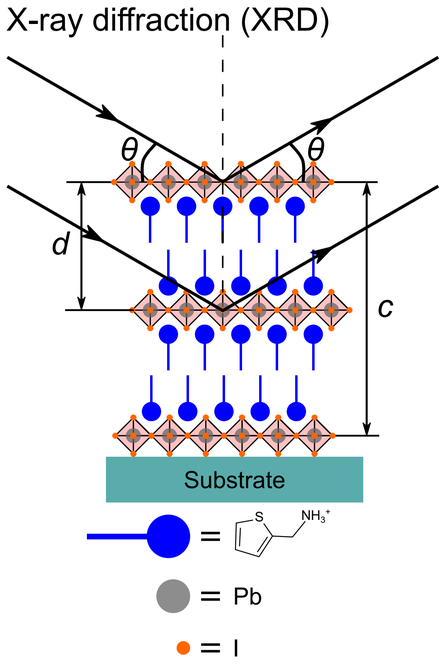
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Introduction

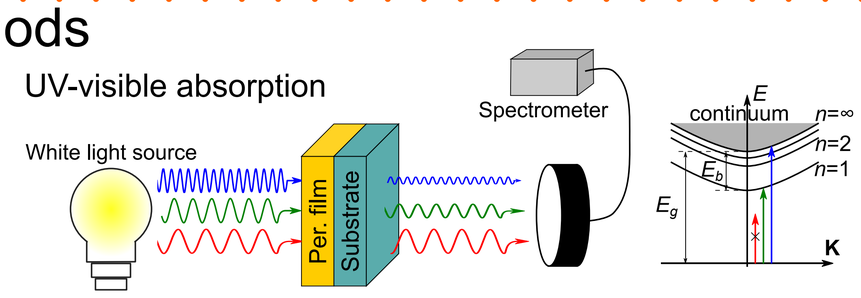
Metal halide perovskites are known for their outstanding optoelectronical properties, such as high charge-carrier mobilities and lifetimes [1, 2] and applications in photovoltaics, light-emitting diodes, photodetectors [3]. Two-dimensional (2D) layered perovskites use long A-site cations to separate adjacent metal halide octahedra sheets, which introduces quantum confinement and allows formation of excitons, giving potential for light-emitting applications. Temperature-dependent studies of perovskite-based devices provide fundamental information on optoelectronic properties, which impact performance and they are important to consider when designing the device. In this work, we study the changes of charge carrier properties in 2D-layered perovskite, 2-thiophenemethylammonium lead iodide ($ThMA_2PbI_4$), caused by temperature-induced structural phase transitions.

Experimental methods

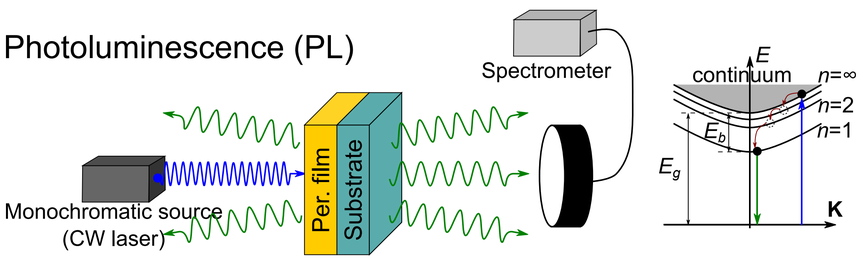
X-ray diffraction (XRD)



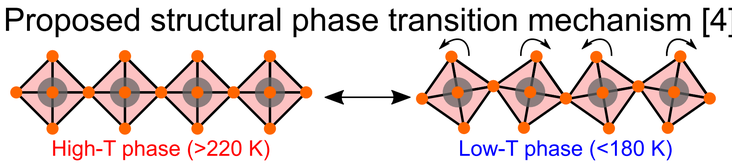
UV-visible absorption



Photoluminescence (PL)

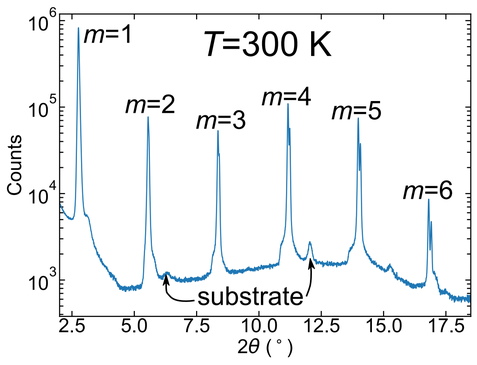


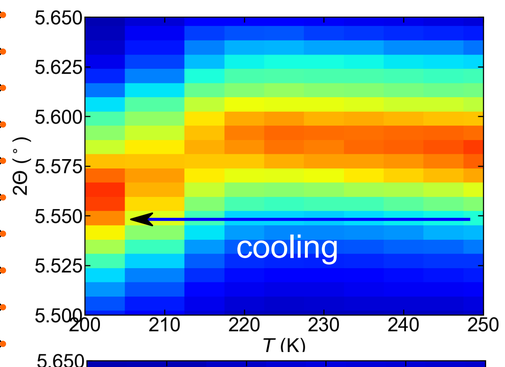
Proposed structural phase transition mechanism [4]

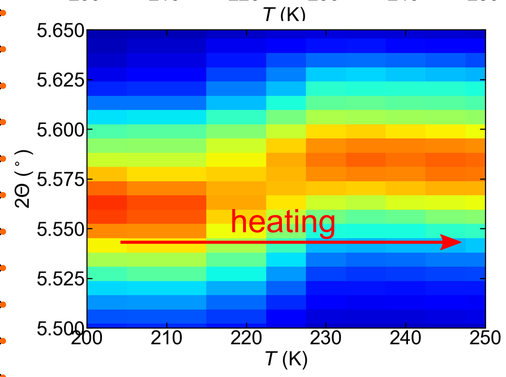


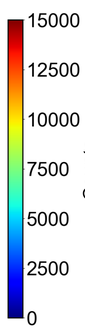
Results

Confirming film orientation and identifying phase transition to the 1st-order

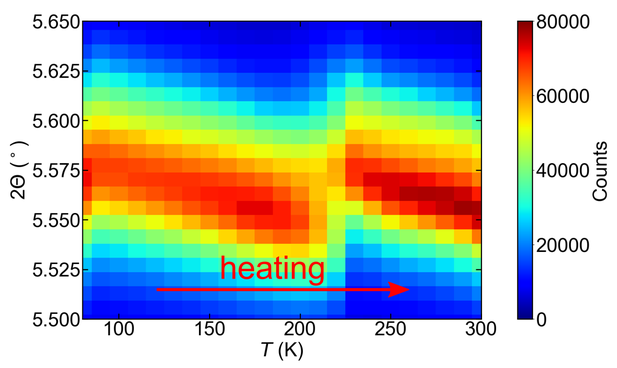


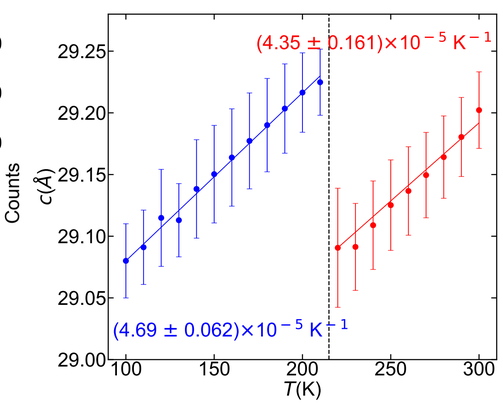




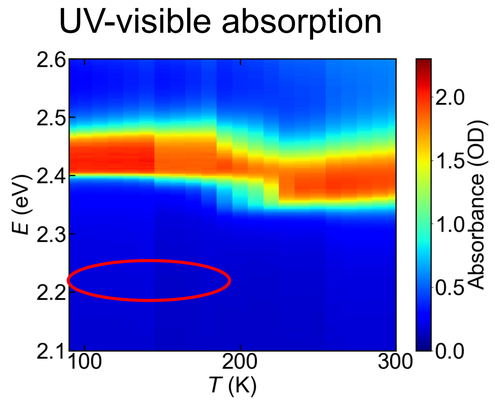


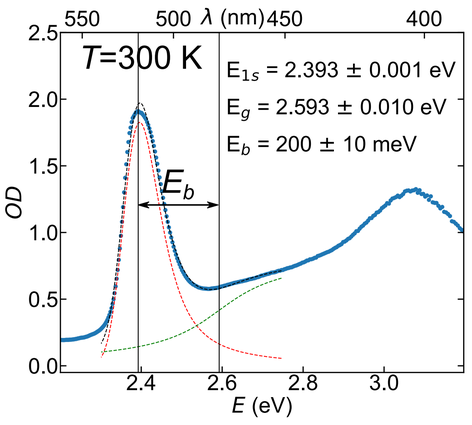
Temperature-dependent XRD, lattice parameters and thermal expansion coefficient

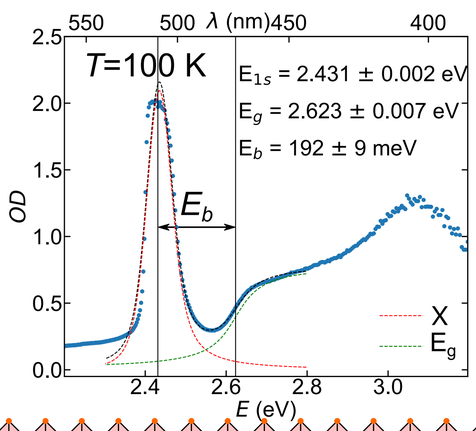




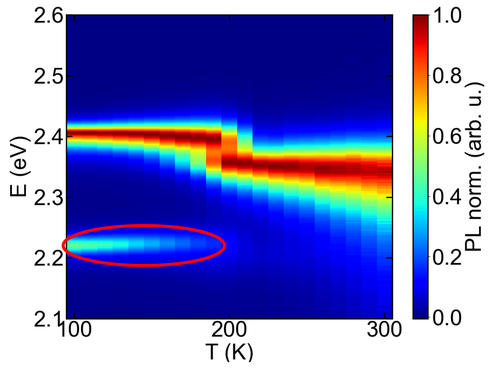
Temperature-dependent UV-visible absorption

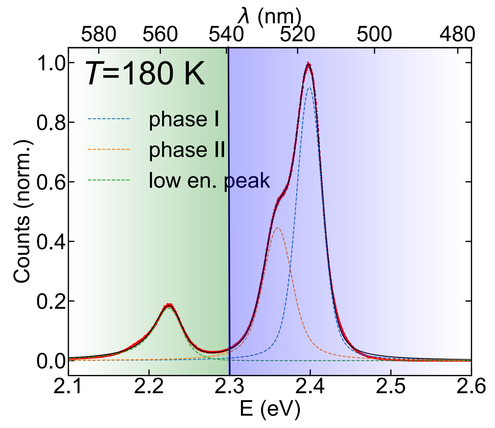




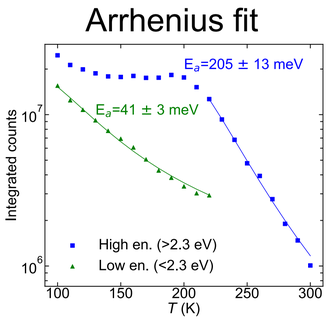


Temperature-dependent PL and analysis of additional PL peak emerging at low T

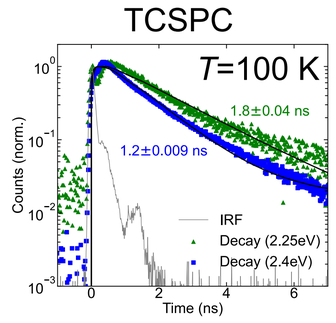




Arrhenius fit



TCSPC



Conclusions

1. We demonstrated that structural phase transition in 2D-layered Ruddlesden Popper perovskite $ThMA_2PbI_4$ affected the distance between metal halide layers and this in turn altered optoelectronic properties by red-shifting both photoluminescence peak and excitonic ground state absorption peak as the sample was heated.
2. The proposed mechanism to explain the phase transition was the metal halide octahedra rotation, altering atomic orbitals of inorganic lattice affecting electronic band structure [4].
3. Additional photoluminescence peak emerging at temperatures below 220 K, but it was absent in UV-visible absorption data. We assigned it to the exciton recombination bound to defects. Further analysis to understand the defect may be beneficial in light-emitting applications.

References

[1] M. B. Johnston and L. M. Herz. *Accounts of Chemical Research*, 49:146–154, 1 2016.
[2] L. M. Herz. *ACS Energy Letters*, 2:1539–1548, 2017.
[3] A. K. Jena, A. Kulkarni, and T. Miyasaka. *Chemical Reviews*, 119:3036–3103, 3 2019.
[4] D. G. Billing and A. Lemmerer (2007). Acta Crystallographica Section B: Structural Science, 63(5), 735–747.

Acknowledgements

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