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The effect of Cs content on the structural and photo physical properties in mixed cation hybrid-perovskites.

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Hybrid-perovskite solar cells have shown rapid development over the last decade reaching 25.2% efficiency in 2019 [1]. Their commercialization is precluded by device stability. The use of mixed cations to substitute the A-site cation site in the prototypical MAPbX3 has shown to greatly improve stability, tune the bandgap and modify the microstructure of the photoactive layer towards a more optimal device. [2][3][4]. A better understanding of the substitution effects on structure and the associated changes in device stability is fundamental in the development and commercialization of these devices.

In the context of phase stabilization, our work investigates the structural, photo-physical and electronic properties of these hybrid-perovskites using both variable-temperature in-situ XRD and time resolved in-situ photoluminescence measurements. Various methods of analysis of the diffraction data are used focusing on sequential and parametric Rietveld refinements along with Pawley fits to extract unit cell parameters, bond lengths, structural distortions and polyhedral orientations for the metal halide framework of the hybrid-perovskites. The inclusion of MA suppresses the formation of the perovskite gamma phase while the inclusion of both MA and Cs changes features of the alpha/beta phase transition.

[1] https://www.nrel.gov/pv/assets/images/efficiency-chart.png, accessed on 2019-10-15
[2] Boyd, C.C., Cheacharoen, R., Leijtens, T. and McGehee, M.D., 2018. Understanding degradation mechanisms and improving stability of perovskite photovoltaics. Chemical reviews, 119(5), pp.3418-3451.
[3] Singh, T. and Miyasaka, T., 2018. Stabilizing the efficiency beyond 20% with a mixed cation perovskite solar cell fabricated in ambient air under controlled humidity. Advanced Energy Materials, 8(3), p.1700677.
[4] Xu, F., Zhang, T., Li, G. and Zhao, Y., 2017. Mixed cation hybrid lead halide perovskites with enhanced performance and stability. Journal of Materials Chemistry A, 5(23), pp.11450-11461.

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