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Probing a Novel Low Temperature State in Cs2AgBiBr6 via Resonance Raman Spectroscopy and Photoluminescence

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Halide double perovskites are of interest due to their potential as high efficiency solar cell materials while eliminating toxicity and stability issues that affect current high efficiency perovskites[1]. Within this family, Cs2AgBiBr6 has advantageous characteristics as a solar cell material including strong absorption and long carrier lifetimes[2]. While a cubic to tetragonal structural phase transition upon lowering temperature to 120 K has been well-documented, there is another characteristic temperature near 40 K. Recent investigations involving the use of temperature dependent neutron and X-ray scattering suggest this phase transition to be due to a complex ground state comprised of a several hundred atom unit cell with elaborate rotations of the silver and bismuth octahedral groups[3]. We have employed optical and thermal techniques to further understand this low temperature phase transition and the impact it has on the optoelectronic properties responsible for the photovoltaic efficiency. Through polarized resonance enhanced Raman spectroscopy, the temperature dependence of the photoluminescence can be analyzed by fitting measured spectra to a series of Voight oscillators. The oscillator fitting parameters show a strong blue shift in the bandgap and deviate from the typical semiconducting exciton linewidth trend. In addition, the A1g/Ag phonon displays a hardening of the center frequency below 40 K. The investigation into this low temperature phase will aid in further developing the understanding of the optoelectronic properties of Cs2AgBiBr6 and similar halide double perovskites.

[1] F. Igbari et al. Advanced energy materials 2019. 9 (12), 1803150.
[2] A. H. Slavney et.al. Journal of the American Chemical Society 2016. 138 (7), 2138-2141.
[3] He, Xing, et al. arXiv preprint 2021. arXiv:2112.04717.

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