Optical Emission of Cs$_2$TiBr$_6$

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Photoluminescence from Single-Crystal and Thin-Film Cs$_2$TiBr$_6$

- Single-crystal and thin-film Cs$_2$TiBr$_6$ exhibit broad PL that can be deconvolved into multiple peaks
- Largest photoluminescence peak at ~2.13 eV is above the bulk 1.8–1.9 eV band gap
- Above $E_g$ PL observed previously in other inorganic perovskites CsPbCl$_3$ and CsPbBr$_3$ and attributed to an exciton bound to a higher-lying defect state within the conduction band
- Near band gap emission also observed
- Lower energy band in thin film spectra is likely defect- and grain-boundary related
- Radiative carrier lifetime is shorter in a thin film due to recombination at defects and grain boundaries
- Single crystal: emission linear in excitation fluence
- Thin film: emission intensity shows saturation as available states fill

Cs$_2$TiBr$_6$: a sustainable solar cell alternative

- ~1.8 eV band gap
- Non-toxic components
- Earth abundant
- Inexpensive
- Extremely air sensitive

Thin-film Fabrication
1. Spin CsBr onto quartz substrate
2. React with TiBr$_4$ vapor at 200 °C

Single-crystal Fabrication
1. CsBr and TiBr$_4$ in a quartz tube in vacuo.
2. Heated in furnace.
3. Crystal facet cleaved with a razor blade.

Cs$_2$TiBr$_6$ is unstable in air, requires atmospheric isolation for PL

Acquisition Details and Future Work

Photoluminescence Spectroscopy:
- 485 nm, ~50 ps pulses focused with 50× objective
- Horiba HR850 spectrometer and Horiba Synchrony CCD spectral resolution
- Time-correlated single photon counting (TCSPC) with Aurea avalanche photodiode single photon detector for time-resolved PL

Future Studies:
- Improve stability of sealed samples by encapsulating sample with TiO$_2$
- Compare optical spectra to DFT calculations of band structure to identify origin of emission

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