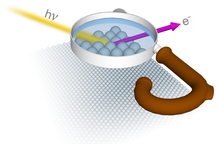
Optical Emission of Cs_2TiBr_6

Emma J. Pellerin,** Emma Burton,*# Maranda Allen,* Caroline Jaeger,*
Erika Colin-Ulloa,* Julia L. Martin,** Lyubov V. Titova,* Ronald L. Grimm**

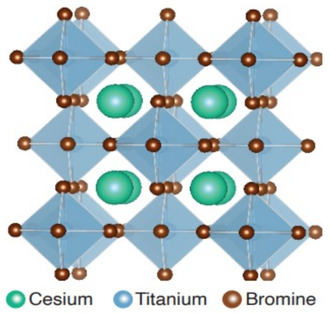
Departments of *Physics and of **Chemistry & Biochemistry, Worcester Polytechnic Institute
 # Department of Physics, Goshen College, Goshen, IN

WPI Ultrafast
THz & Optical Spectroscopy Lab



WPI

GOSHEN COLLEGE



Cs_2TiBr_6: a sustainable solar cell alternative

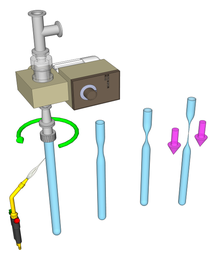
- ~1.8 eV band gap
- Non-toxic components
- Earth abundant
- Inexpensive
- Extremely air sensitive

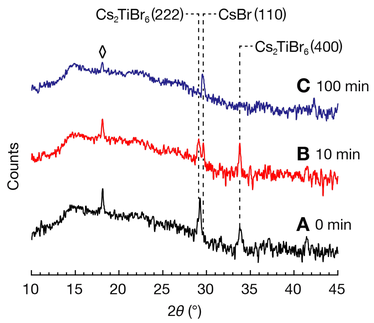
Thin-film Fabrication

1. Spin CsBr onto quartz substrate
2. React with $TiBr_4$ vapor at 200 °C

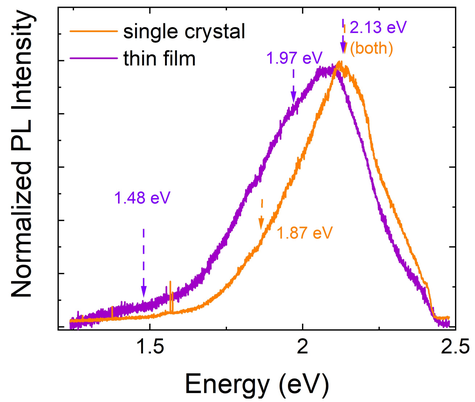
Single-crystal Fabrication

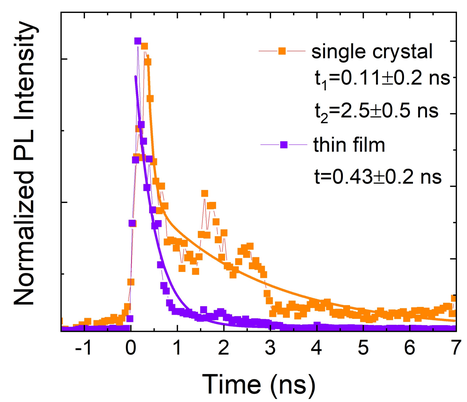
1. CsBr and $TiBr_4$ in a quartz tube in vacuo.
2. Heated in furnace.
3. Crystal facet cleaved with a razor blade.

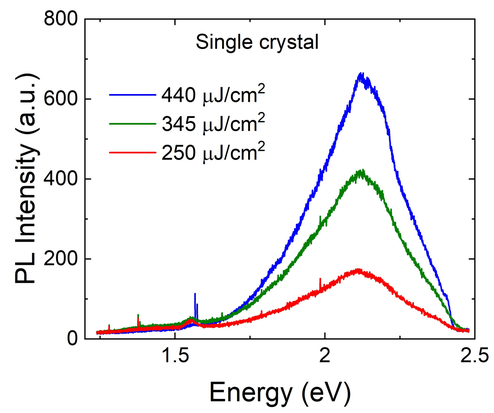


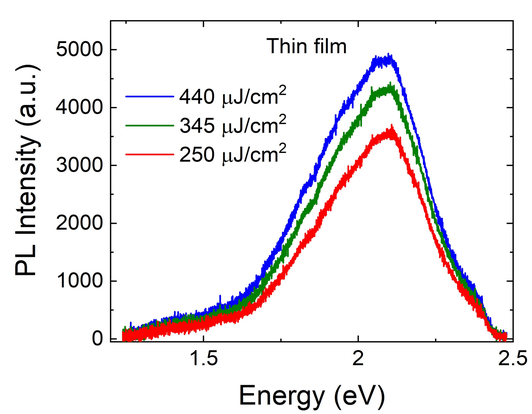


Cs_2TiBr_6 is unstable in air, requires atmospheric isolation for PL









Photoluminescence from Single-Crystal and Thin-Film Cs_2TiBr_6

- Single-crystal and thin-film Cs_2TiBr_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 [3]
- 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

Acquisition Details and Future Work

Photoluminescence Spectroscopy:

- 485 nm, ~50 ps pulses focused with 50× objective
- Horiba iHR550 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

References & Acknowledgements

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2. J. L. Mendes, W. Gao, J. Martin, A. Carl, N. Aaron Deskins, S. Granados-Focil, and R. L. Grimm, *J. Phys. Chem. C*, **2020**, *124*, 24289-24297.
3. M. Sebastian, et alii, *Phys. Rev. B* **2015**, *92*, 235210.

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