

# Bismuth Triiodide ( $\text{BiI}_3$ ) – A Candidate Photovoltaic Absorber

## Scientific Achievement

We identified  $\text{BiI}_3$  as a candidate photovoltaic absorber using computational design criteria based on the methyl ammonium lead iodide perovskites. Initial experiments demonstrate room-temperature photoluminescence with application-relevant lifetimes.

## Significance and Impact

New materials are needed for high-performance, low-toxicity, Earth-abundant photovoltaic absorbers. We employed Materials-by-Design methods to first predict and then experimentally verify the promise of  $\text{BiI}_3$ .

## Research Details

- Computed electronic structure via first principles (Fig. 1b).
- Physical vapor transport and spin-coating of thin films. Bridgman-style growth of single crystals.
- Measured optical absorption and photoluminescence.
- Measured carrier recombination time constant using time-resolved photoluminescence (Fig. 2).
- Carrier lifetimes  $\sim 180$  ps in thin films and  $\sim 1.5$  ns in single crystals.

R.E. Brandt et al., *J. Phys. Chem. Lett.* **6**, 4297 (2015).

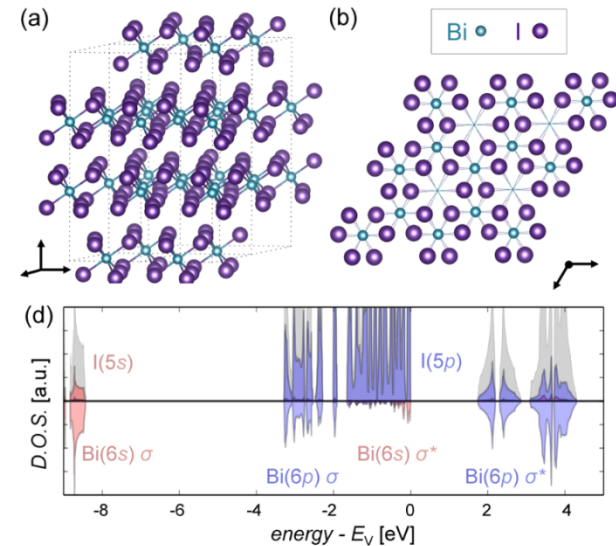


Fig. 1: (top) Crystal structure of  $\text{BiI}_3$ . (bottom) Calculated electronic density of states.

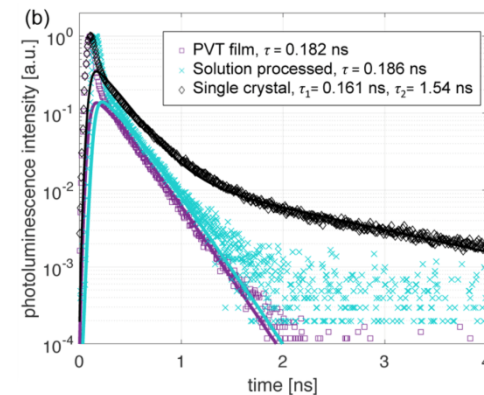


Fig. 2: Measurements of carrier lifetime by Time-resolved photoluminescence.