

Bismuth Triiodide (BiI_3) – A Candidate Photovoltaic Absorber

Scientific Achievement

We identified 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 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 ~ 180 ps in thin films and ~ 1.5 ns in single crystals.

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

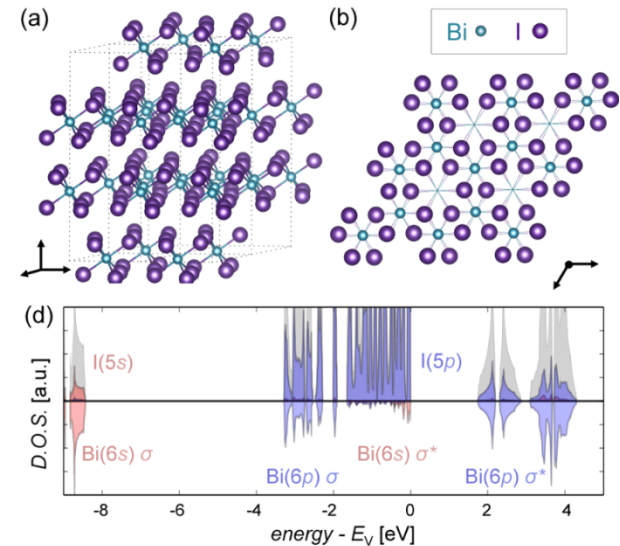


Fig. 1: (top) Crystal structure of BiI_3 . (bottom) Calculated electronic density of states.

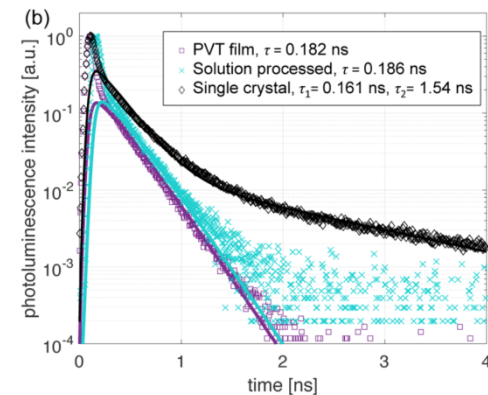


Fig. 2: Measurements of carrier lifetime by Time-resolved photoluminescence.