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).
– 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.