Washington University in St. Louis
Office of Technology Management

STABLE, NON-TOXIC LEAD-FREE PEROVSKITE MATERIALS FOR HIGH EFFICIENCY SOLAR CELLS AND OTHER SEMICONDUCTOR APPLICATIONS

Biswas, Pratim, Kavadiya, Shalinee, Mishra, Rohan, Thind, Arashdeep Singh

Carter, Paul

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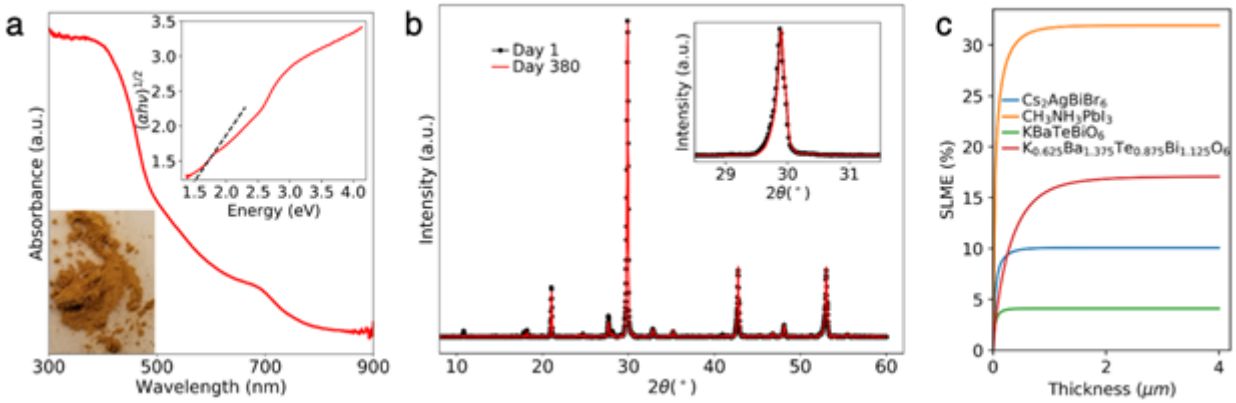
Engineers at Washington University in St. Louis have discovered a new class of stable, benign perovskite semiconductor materials with performance properties optimized for solar cell and photocatalysis applications. Traditional lead-halide perovskites show remarkable power conversion efficiency in photovoltaic applications. However, they are intrinsically unstable and contain toxic lead which can contaminate the environment and cause chronic health issues. This technology addresses those problems by replacing lead with non-toxic bismuth to create a defect-tolerant, inorganic double perovskite oxide semiconductor material without compromising its semiconductor properties.

Using a material informatics approach, the inventors designed a previously unknown compound they predicted would be thermodynamically stable and have high optical absorbance, small effective mass of carriers, and optimal band gap for semiconductors. Subsequent synthesis and experimental testing of this lead-free compound confirmed a band gap of 1.5eV and excellent stability. Additional materials with the general stoichiometry of this lead-free compound could provide exciting benign alternatives to lead-halide perovskites, opening the untapped potential of inorganic bismuth-based double perovskite oxides for semiconductor applications such as photovoltaic cells, photocatalysis and optoelectronics.



Experimental stability and theoretically predicted absorbance of Bi perovskite: ***(a)*** *Material had experimental band gap of 1.5 eV and* ***(b)*** *was stable under ambient conditions.* ***(c)*** *Its theoretically predicted efficiency as a solar absorber compares favorably to promising halide perovskites.*

Stage of Research

The inventors have successfully synthesized a candidate bismuth double perovskite with wet chemistry and demonstrated experimental indirect band gap of 1.5 eV with stable absorption over time. Their continued research includes testing the material on a solar cell for carrier mobility and efficiency.

Applications

- **Solar cells** – high performance absorber layer
- **Photocatalysis**

Key Advantages

- **High performance:**
  - optimal band gap (experimental indirect band gap of 1.5eV, comparable to the best performing halide perovskites)
  - simulations predict favorable charge transport
  - comparable effective masses of charge carriers to prototype lead-halide perovskites
- **Stable –** maintains performance under ambient conditions, unlike conventional lead-halide perovskites where efficiency degrades within a few days
- **Non-toxic material –** bismuth-based material is environmentally benign, unlike conventional perovskites which contain toxic lead

Patents

- Provisional patent application filed

Website

- Materials Modeling and Microscopy (M-cube) group
- Aerosol and Air Quality Research Laboratory