

Identifying Defect-Tolerant, High-Lifetime Semiconductors

Scientific Achievement

The key role that band-edge orbital character has on defect tolerance (gained from MAPbX_3 perovskites) underlies a new joint data-mining and theory approach to screen materials for long minority-carrier lifetimes, which is a critical photovoltaic (PV) absorber property.

Significance and Impact

We have identified inorganic PV absorber materials with potential MAPbX_3 -like performance but improved stability.

Research Details

- **Screening Criteria:** Key material parameters that distinguish MAPbX_3 are antibonding orbital character of both the conduction and valence band extrema (Fig. 1), small effective masses, and large static dielectric constant.
- **Screening Tools:** Using these “defining parameters,” 27,000 inorganic semiconducting materials from the Materials Project were evaluated and a few dozen identified as promising (Fig. 2).
- **Next Steps:** Investigate electronic structure of potential novel PV absorbers and synthesize promising candidates.

R. Brandt, V. Stevanovic, D. Ginley, T. Buonassisi, *MRS Comm.*, DOI:10.1557/mrc.2015.26 (2015).

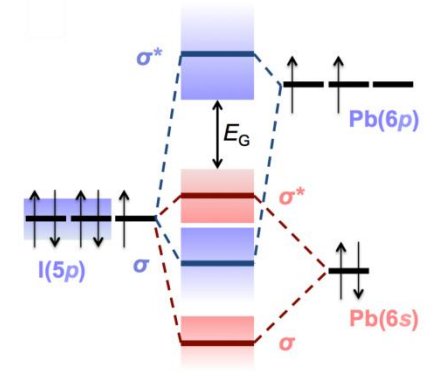


Fig. 1. Orbital character of band edges in MAPbI_3 .

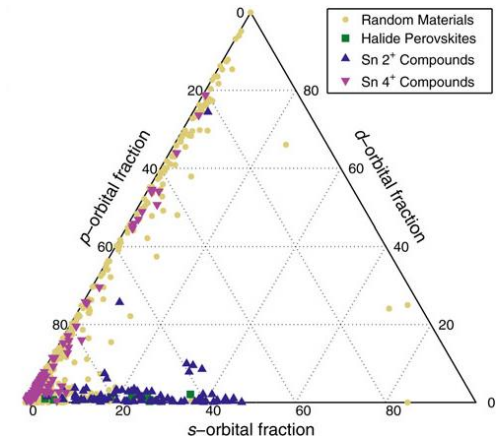


Fig. 2. Orbital type at valence band maximum.