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.

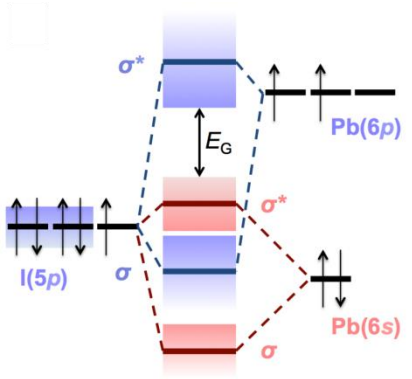

Fig. 1. Orbital character of band edges in $MAPbI_3$.

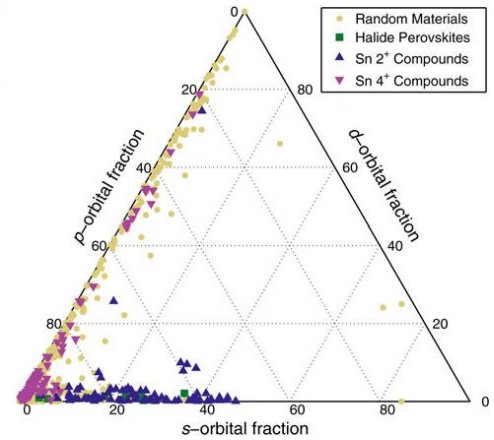

Fig. 2. Orbital type at valence band maximum.

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

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