Design Principles Demonstrated for Semiconducting d^5 Transition-Metal Oxides with Photovoltaic Applications Potential

Scientific Achievement

The Center for Inverse Design (CID) used theory to predict band structure and transport properties for the d^5 transition metal (TM) oxides MnO and Fe_2O_3.

Significance and Impact

This work identified design principles for improving d^5 oxides as a new class of semiconductors with potential applications in energy conversion.

Research Details

- ***Computational methods***: Many-body GW calculations and *ab-initio* polaron theory for Fe_2O_3 and two modifications of MnO (RS, rock-salt; and ZB, zinc-blende).
- ***Band structure***: Theory shows electronic structure of d^5 oxides leads to desirable low effective masses; in addition, zinc-blende MnO has a bandgap in visible range.
- ***Carrier self-trapping***: Mn tends to trap holes, Fe tends to trap electrons; hole trapping (small-polaron) can be avoided by the tetrahedral coordination in ZB-MnO.
- ***Outlook***: This work is the basis for further materials design of d^5 oxides: ternary compounds and alloys.

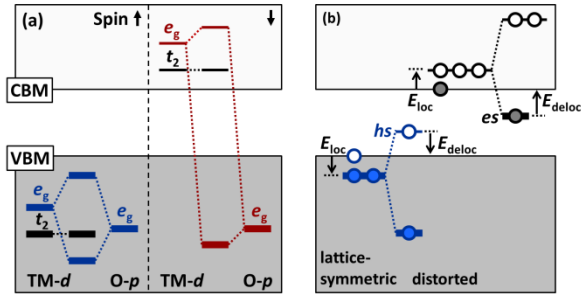

Figure 1: Schematic illustration of the (a) atomic orbital interaction in d^5 oxides, and (b) formation of a self-trapped hole state (*hs*) or electron state (*es*).

Table: Bandgap E_g (eV), effective mass m^* (in units of m_e), and self-trapping energy E_{ST} (eV) for electrons (e) and holes (h).

	E_g	m_e^*	m_h^*	E_{ST} (h)	E_{ST} (e)
RS-MnO	3.4	0.3	1.2	−0.24	–
ZB-MnO	2.1	0.3	4.8	+0.23	–
Fe_2O_3	2.0	1.5	2.1	–	−0.23

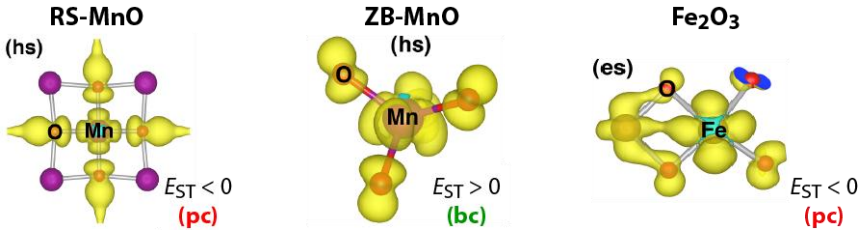

Figure 2: Wave-functions of the self-trapped (small-polaron) state; sign of E_{ST} indicates band or polaron conduction (bc or pc).

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Work performed at the National Renewable Energy Laboratory

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