Transition Metal Oxide Semiconductors

Scientific Achievement

Comprehensive assessment of semiconducting transition metal oxides using unbiased electronic structure calculations with integrated treatment of s, p, and d electrons.

Significance and Impact

Demonstrated that transition metal oxides can be viable semiconductors amenable to theory-guided Materials by Design despite the possible presence of correlated electron effects and a Mott gap.

Research Details

- Electronic structure calculations for transition metal oxides within a uniform GW approach.
- Electronic trends and semiconducting properties of the binary 3d oxides.
- Rigorous approach for distinguishing band-like and small polaron (hopping) conduction.
- Complex defect physics in transition metal oxides.
- 300+ GW band-structure calculations at <u>http://materials.nrel.gov</u>
- S. Lany, J. Phys.: Cond. Matter 27, 283203 (2015)



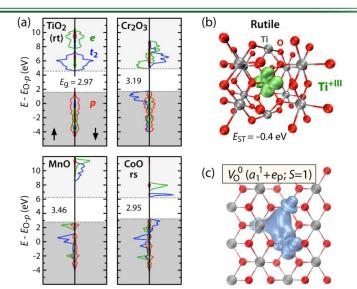


Fig. 1: (a) Electronic density of states. (b) Small polaron. (c) Complex defect states.

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quiro id 320 238	ed elements: [<mark>sorted formula</mark>	<mark>final SG</mark> 227	ΔEcbm 1.138 1.602	ΔEvbm -1.420 -1.455	Elements: ^{F_e(TDDFT) 2.960}	E _g (eV)	<mark>E_{g,d} (eV)</mark> 5.716	me*/m0	m _h */m ₀	standards	<mark>parents</mark> [9340] [9367]	Family
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Fig. 2: The NREL Materials Database contains 300+ GW band-structure calculations.

HARVARD

