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 http://materials.nrel.gov

S. Lany, *J. Phys.: Cond. Matter* **27**, 283203 (2015)

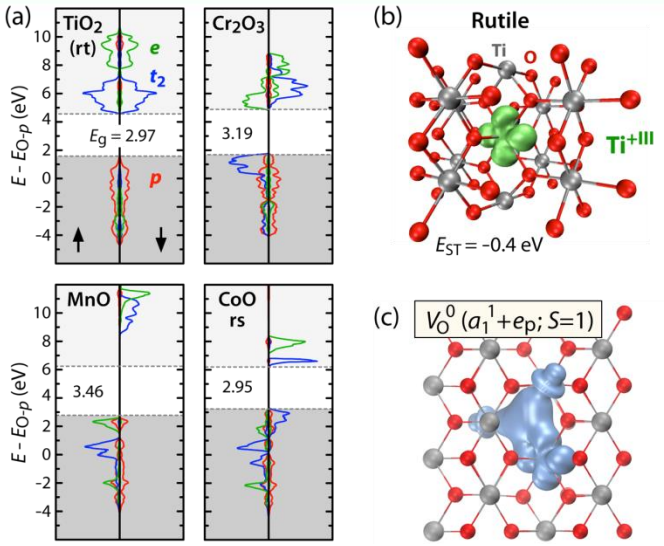

Fig. 1: (a) Electronic density of states. (b) Small polaron. (c) Complex defect states.

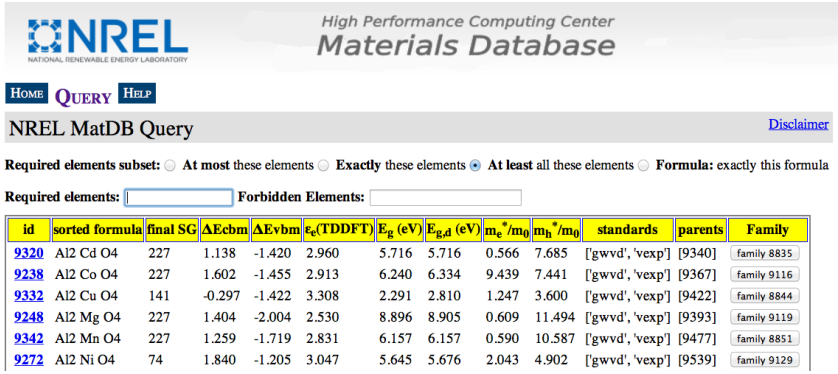

Fig. 2: The NREL Materials Database contains 300+ GW band-structure calculations.