**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.


**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.