Accurate Band-Structure Calculations for the 3*d* Transition Metal Oxides

Scientific Achievement

The Center for Inverse Design has developed a method to calculate accurate band structures and bandgap energies for *3d* transition metal oxides using an augmented GW formalism.

Significance and Impact

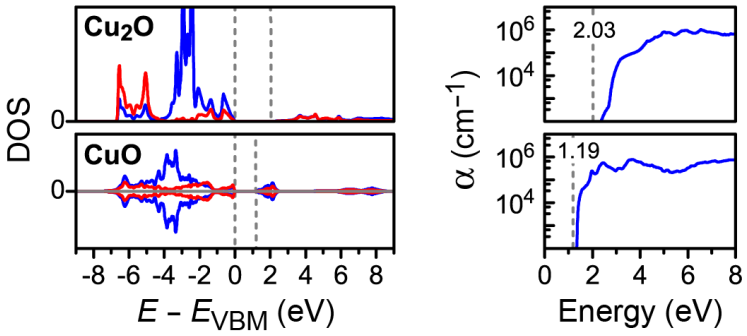
This approach provides a computationally viable route for high-throughput prediction of band structures and optical properties in transition metal compounds.

E_g [eV]	Expt.	GW_{RPA}	GW_{Vd}
TiO_2	3.0	4.48	3.11
Cr_2O_3	3.2	4.75	3.23
FeO	2.1	1.65	2.14
Fe_2O_3	2.1	3.57	2.01
Cu_2O	2.1	1.59	2.03
CuO	1.6	2.49	1.19

Bandgaps E_g (eV) in experiment, in standard GW (RPA), and in the new GW with V_d potential method.

Research Details

- Many-body GW calculations are accurate for main-group compounds, but not for transition-metal compounds.
- We have shown that using an element-specific on-site potential for transition-metal *d*-orbitals can qualitatively improve the calculated bandgap energies (see table).
- Using this method, electronic structure calculations with correct *d*-band energies and accurate absorption spectra can be calculated (see figure).
- This will enable high-throughput band-structure prediction for semiconductor materials containing transition metals.



Density of states (DOS) and absorption spectrum, shown for Cu_2O and CuO.

S. Lany, *Phys. Rev. B* **87**, 085112 (2013).