Scientific Achievement

ZnO is an important prototypical wide-gap oxide semiconductor. The discrepancy between band-structure theory and ARPES is removed by a correction for the Zn-\(d\) band energy in GW calculations.

Significance and Impact

The present approach improves the capability for property prediction and design of energy materials.

Research Details

- **Experiment:** ARPES measurements of the valence band structure provide reference data with unprecedented resolution.
- **Theory:** Band-structure calculations show that the \(d\)-band energy is considerably overestimated in common approaches. Application of an on-site potential for Zn-\(d\) states is suggested as a solution. The approach can be extended to other materials, and it improves the prediction of defect energies, band offsets, and ionization potentials.


Work performed at SLAC, NREL, and CU Boulder