Benchmarking Band-Structure Calculations Against Angular-Resolved Photoemission Spectroscopy (ARPES) for ZnO

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.

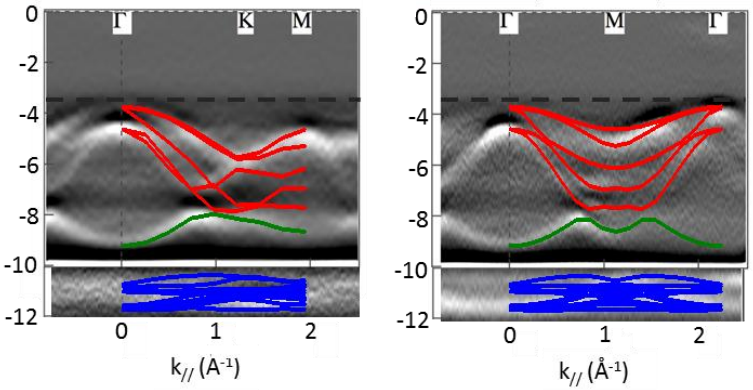

Figure 1: ZnO valence band structure in ARPES spectra (gray scale) and GW band-structure calculations (lines) that include an on-site potential to correct the energy of the Zn-*d* band (blue).

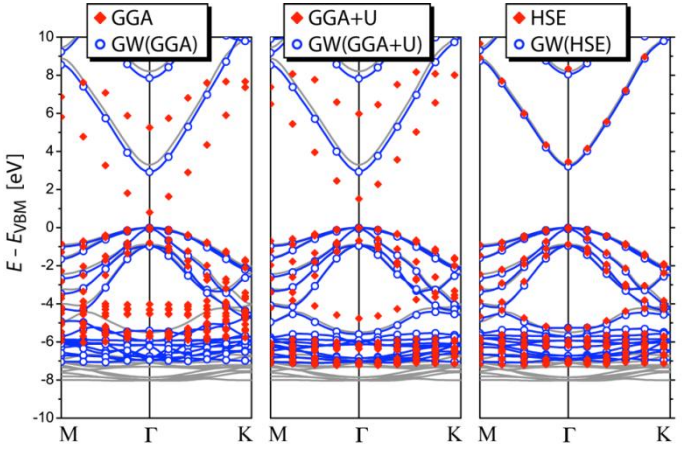

Figure 2: Band-structure calculations for ZnO, showing that the error in the *d*-band energy occurs for different functionals used to generate the wavefunctions.

L.Y. Lim, S. Lany, Y.J. Chang, E. Rotenberg, A. Zunger, M.F. Toney, *Angle-resolved photoemission and quasiparticle calculation of ZnO: The need for d band shift in oxide semiconductors, Phys. Rev. B* **86**, 235113 (2012) DOI: 10.1103/PhysRevB.86.235113

Work performed at SLAC, NREL, and CU Boulder

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