Optical Properties of $Zn_2Mo_3O_8$: GW+BSE Study (PV-3)

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Scientific Achievement:

We computed the DFT band structure and orbital-resolved density of states for ZMO. Quasiparticle corrections have also been included within G_0W_0 approximation. To obtain absorption spectra, we solved the Bethe-Salpeter equation, which is a state-of-the-art methodology that captures electron-hole interactions as well.

Significance and Impact:

DFT calculation, which usually underestimates the bandgap, suggests that the material is an indirect-gap semiconductor with a gap of 1.67 eV. Quasiparticle corrections increase the gap to 3.14 eV. After solving the BSE equation, we found that the lowest exciton is at 2.38 eV. Our calculation shows that the material has a huge exciton binding energy of 0.78 eV; hence, it may not be suitable for photovoltaic applications.

Research Details:

- DFT calculations were performed using the Quantum Espresso package, which uses a plane-wave basis set.
- GW+BSE calculations were performed using the BerkeleyGW package.

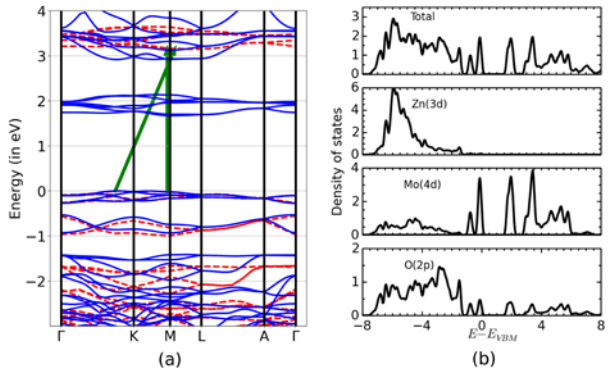

Fig. 1: DFT-GW band structure and orbital-resolved density of states of ZMO.

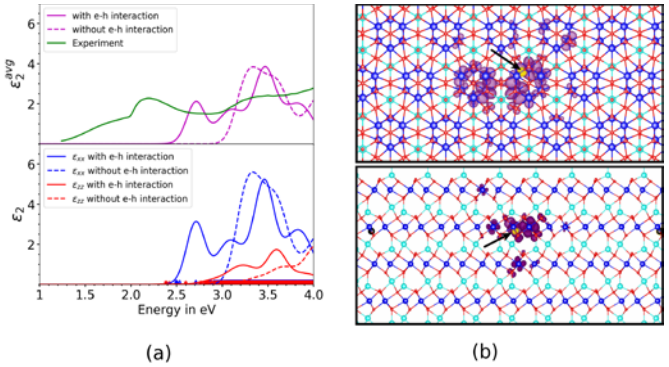

Fig. 2: Imaginary part of the dielectric function and lowest-energy exciton wavefunction.

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