Assigning Spectral Features in Excitonic Spectra

ERIC L. SHIRLEY, NIST — Considerable progress has been made over the last several years in calculations of optical absorption spectra from first principles. This builds on the foundation of accurate electronic band structures, including many-body corrections to band energies, and realistic solution of the couple equation of motion for an electron-hole pair in the excited state. Omitting the electron-hole interaction (or excitonic effects) can severely hamper the accuracy of a spectrum. In narrow-gap semiconductors (Si, Ge, GaAs, etc.), this is a reasonably tolerable situation, in the sense that assigning spectral features can be (and has been) used to establish energies of interband transitions at critical points. In wider gap systems, such as LiF or MgO, the qualitative change in spectral features resulting from electron-hole interactions might call into question assignment of features to interband transitions. This talk presents an attempt to carry out such assignments, nonetheless.