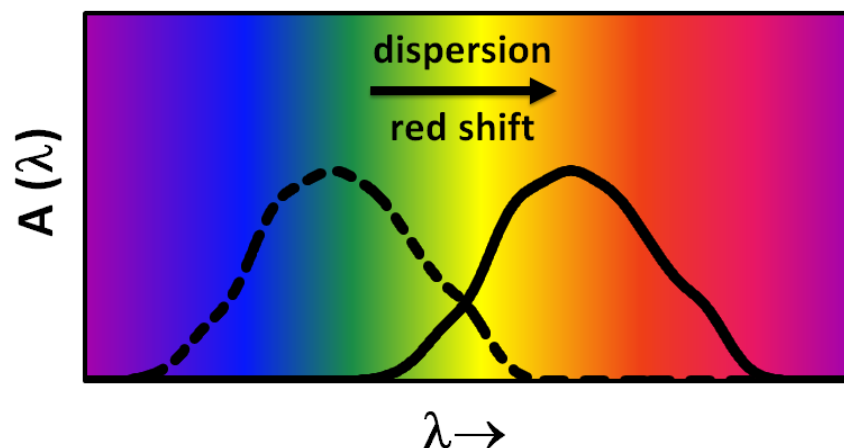
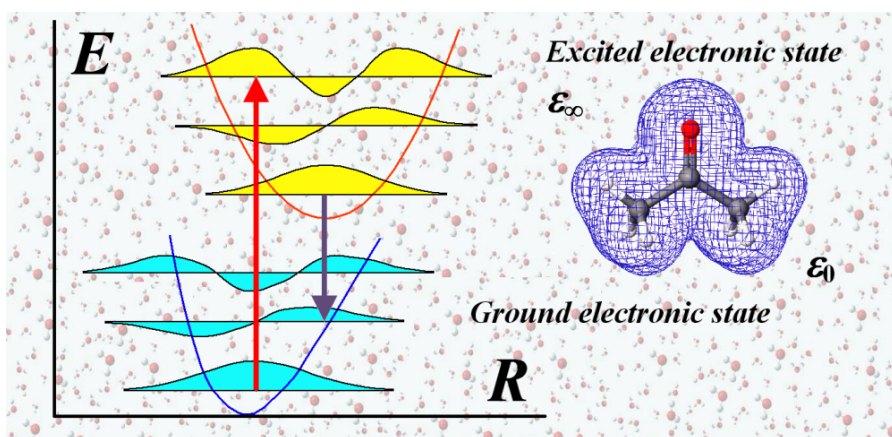


# Medium Effects on Excited-State Energy Surfaces



Reference: A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Chem. Theory Comput.* 2013, 9, 3649.

Work was performed at Department of Chemistry, Chemical Theory Center, and Supercomputing Institute, University of Minnesota.

## Scientific achievement

We present a new efficient treatment of solute–solvent dispersion contribution to solvatochromic shifts based on state-specific polarizability.

## Significance and Impact

One can now compute vertical excitation and emission spectra in solution more realistically.

## Research Details

- The model uses only two descriptors, namely, the averaged molecular dipole polarizability of the solute and the refractive index of the solvent.
- It efficiently predicts solvatochromic shifts for a number of systems where solute–solvent dispersion dominates the observed shift.
- We have incorporated this model into our open-source code VEMGAUSS to combine a state-specific treatment of the solvent polarization with a state-specific treatment of dispersion.