Molecular Vibronic Spectra in Solution Simulated by Damped Franck-Condon Factors

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Abstract

Franck-Condon factors bridge the gap between theoretical modeling and experimental observations for molecular electronic spectroscopy and electron transfer. Under the displaced harmonic oscillator approximation, multidimensional Franck-Condon factors are decomposed into a product of many one-dimensional (1D) Franck-Condon (FC) factors, which are successfully applied to simulate molecular vibronic spectra in gases phase. For dealing with simulation of the spectra in solution, various ab. initio methods, such as polarizable continuum model (PCM) and explicit solvent model, added correction in static interactions between solute and solvent molecules. However, how to treat dynamic correction to the spectra is not well-studied. We have recently developed the dynamic correction method leading to direct modification of Franck-Condon factors by damped oscillators. This method was applied to simulate absorption and fluorescence spectra of perylene, isoquinoline, rubrene molecule in solutions. The present simulation presents nice physical insights for dynamic correction to solvent-enhanced vibronic spectra.

References

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