TIME-DEPENDENT DFT CALCULATIONS FOR EXCITATION SPECTRA OF PORPHYRINES AND PHTHALOCYANINES

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The time-dependent DFT method affords an efficient method for the calculation of excitation spectra. The response calculations require an accurate Kohn-Sham potential, including the exchange-correlation part, and an accurate exchange-correlation kernel. It will be demonstrated that the quality of the Kohn-Sham is crucial to obtain highly accurate results. Proper asymptotic behaviour as well as proper behaviour in the valence and core electron regions (intershell steps) is important. The quality of the XC kernel is not so critical.

We will apply the TDDFT method to the calculation of porphyrine and phthalocyanine spectra. An KS orbital interpretation of the well-known Q and B band system will be given, including a critical discussion of the time-honoured cyclic polyene mpdel for porphyrine spectra. The interpretation of recent MCD spectra is also addressed.