Theoretical approaches for predicting the color of rigid dyes in solution

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Aiming at developing an affordable and easily implementable computational protocol for routine prediction of spectral properties of rigid molecular dyes [1], a computational approach based on DFT and TD-DFT in conjunction with a vibronic treatment for band shape prediction and a polarizable continuum model for solvent description is shown to provide good accuracy in perceived colors of structurally rigid molecules considered as prototype for families of dyes of industrial relevance [2]. In order to evaluate the accuracy of the computational protocol proposed not only absorption maxima and band shape profiles were compared but also LAB colorimetric characteristic of the dyes. The latter led to quantitatively evaluate the errors in predicted color and to quantify the sensation of 'difference in color'. The results show that a mixed protocol, implying the use of a global hybrid functional for the prediction of adiabatic energy differences and a range separated hybrid for the prediction of potential energy curvature, allows perceived colors to be quantitatively predicted, as demonstrated by the comparison of L*a*b* colorimetric parameters obtained from computed and experimental spectra [3].

References

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