NONEMPIRICAL SIMULATIONS OF VIBRONIC SPECTRA OF ORGANIC DYES IN SOLUTION

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Abstract: Technological advances trigger the quest for efficient dyes with tailored photophysical properties. Depending on target application, the absorber must meet several criteria, e.g., absorption wavelength must fit into desired spectral window, (multiphoton) absorption cross section should exceed required threshold or there should be an efficient emission from one of electronic excited states. There are on-going efforts to develop cost-effective but reliable computational protocols supporting the design of organic and organometallic systems with desired (multiphoton) absorption cross sections with an eye towards technology-related applications. The aim of the talk is to assess the reliability of electronic-structure theories in nonempirical simulations of electronic (multiphoton) absorption spectra focusing on: *(i)* the performance of time-dependent density functional theory, *(ii)* the importance of non-Condon effects, *(iii)* the accuracy of embedding schemes for estimations of inhomogeneous broadening, *(iv)* the development of machine-learning-based protocols to reduce computational costs. A few case studies will be presented for the members of important classes of fluorescent dyes.

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