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Theoretical description of excited state dynamics in nanostructures[1]

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There has been much progress in the synthesis and characterization of nanostructures however, there remain immense challenges in understanding their properties and interactions with external probes in order to realize their tremendous potential for applications (molecular electronics, nanoscale opto-electronic devices, light harvesting and emitting nanostructures). We will review the recent implementations of TDDFT to study the optical absorption of biological chromophores, one-dimensional polymers and layered materials. In particular we will show the effect of electron-hole attraction in those systems. Applications to the optical properties of solvated nanostructures as well as excited state dynamics in some organic molecules will be used as text cases to illustrate the performance of the approach. Work done in collaboration with A. Castro, M. Marques, X. Andrade, J.L Alonso, Pablo Echenique, L. Wirtz, A. Marini, M. Gruning, C. Rozzi, D. Varsano and E.K.U. Gross.

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