

Ab Initio Colors

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In this talk I will present some recent work addressing the effects of the solvent (water) on the optical properties of natural dyes. I will break the ice with a short presentation of the physics and physiology of color vision, in the style of popular science. I will then introduce *Time-Dependent Density-Functional Perturbation Theory*, a technique allowing for the simulation of the optical spectra of molecular models of up to several hundred (and possibly even a few thousand) inequivalent atoms, without computing any virtual states. This technique will be demonstrated with the “prediction” that grass is green, and applied to the optical properties of flavylum, the dye that gives aubergines and blueberries their typical deep-purple coloration [1]. In the latter case I will show that the main effect of the solvent is to provide a medium allowing thermal fluctuations to fill the gaps that would otherwise characterize the spectrum of the dye at $T = 0$, thus considerably enhancing optical absorption in the visible range.

- [1] O. B. Malcioglu, A. Calzolari, R. Gebauer, D. Varsano, and S. Baroni, *JACS* **133**, 15425 (2011).