A study of the optical properties of a bio-sourced dye

Ilaria Ciofini[1], Carlo Adamo[1], Marco Pagliai[2], Gianni Cardini[2], and Irene Pusceddu[1,2]

[1]*Chimie ParisTech, PSL University, CNRS, Institute of Chemistry for Life and Health Sciences, Theoretical Chemistry and Modeling Team, 75005, Paris, France*
[2]*Dipartimento di Chimica "Ugo Schiff", Università degli Studi di Firenze, Sesto Fiorentino 50019, Italy*
irene.pusceddu@etu.chimieparistech.psl.eu

ABSTRACT

The textile industry is responsible for around 10% of global carbon emissions and 20% of global water pollution each year [1]. With dyeing steps representing a significant portion of the industry's environmental impact, the computational evaluation of a dye's color has the potential to substantially speed up the screening of new dyeing agents with a greener footprint. The study we present offers an example of how such a computational protocol might be implemented. We investigated the optical properties of a bio-sourced dye, derived from anthraquinone, substituted by amino or hydroxyl groups in different positions. With a specific focus on the prediction of the dyes' color in solution, the effects of the solvent and the number, nature, and relative position of these groups on the starting molecule are examined by means of time-dependent density functional theory calculations, used to accurately predict hue, brightness, and color strength over the molecular set.

For each compound, the absorption spectrum within the visible range (1.65 to 3,25 eV) is calculated at PBE0 level in combination with the 6-31++g(2d,2p) basis set. The band shape, the other crucial element for the evaluation of the perceived color, has been simulated by considering the vibronic contributions thanks to the LQ2 approximation [2], a powerful method for rigid dyes like the one under study.

Methanol has been chosen as solvent, as it provides a simple model for cellulose. The polarizable continuum model has initially been used, with a molecule of methanol later added to assess the impact of hydrogen bonds on the perceived color.

The resulting absorption spectra have been then translated into predicted colors by combining the computed spectral shapes with the spectrum of a standard D65 light source and considering their superposition with the set of response functions characterizing the human eye.

References

[1] S Parliament, European. "The impact of textile production and waste on the environment (infographic)." *Retrieved December* 5 (2022): 2022.

[2] Li SL, Truhlar DG. Franck–Condon models for simulating the band shape of electronic absorption spectra. *Journal of Chemical Theory and Computation*. **2017** Jun 13;13(6):2823-30