

## Virtual eyes for technology and cultural heritage: towards computational strategy for new and old indigo-based dyes

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### Streszczenie

A cost-effective, robust and reliable computational strategy is applied to simulate peak positions and band shapes of UV–Vis spectra together with the dye colours perceived by human eyes. The features of our virtual multifrequency spectrometer (VMS) relevant to this topic are sketched with special focus on the selection of density functional, vibronic model and solvent description. Furthermore, the new VMS-draw graphical user interface is employed for user-friendly pre- and post-processing of the computed data. The family of indigo dyes is used as case study in view of their continued use in the field of cultural heritage, together with new promising applications for photonics and sustainable energy. After assessment of different simplified models employed in previous studies, the role of several substituents and of dimerization in tuning the colour and spectral features are analysed in detail by means of both accurate computations and interpretative models. The results are in remarkable agreement with experiment and allow to rationalize the behaviour of this class of dyes.

### Słowa kluczowe

Indigoits, Quantum mechanical calculations, TD-DFT,  
Electronic spectra line shapes

### Adres publiczny

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### Strona internetowa wydawcy

<http://link.springer.com>