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**Modeling the color of natural dyes** XIAOCHUAN GE, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy, ARRIGO CALZOLARI, Centro S3 - CNR-NANO, Modena, Italy, SIMON BINNIE, STEFANO BARONI, Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy — We report on a theoretical study, based on time-dependent density-functional theory, of various factors affecting the optical properties of a few representative anthocyanins, a class of molecules responsible for the color of many fruits, flowers, and leaves, which have also aroused some interest for photovoltaic applications. We first address the influence of substituting different side groups in the phenyl ring of flavylium dyes. We find that these dyes can be classified into three broad classes, according to the number of peaks (1, 2, or 3) featured in the visible range, and give a rationale to this finding. We then examine the effects of solvent-induced thermal fluctuations and dielectric screening, by calculating the spectrum of a representative molecule in solution, for each one these classes. This is achieved by first running an ab initio molecular dynamics simulation of an explicit model for the water-solvated molecule, and then accumulating time averages of the optical spectra calculated on the fly. The effects of thermal fluctuations are shown to overshadow those of dielectric screening, and more dramatic the larger the number of peaks in the gas phase. The effects of different functionals (GGA vs. hybrids) on the calculated spectra are also addressed.

Xiaochuan Ge
Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy

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