Exploring the potential of anthocyanins as a natural dye for non-food applications

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Since the mid-19th century, synthetic dyes, are dominating in many applications such as cosmetics, textile and food colorants. However, these dyes potentially possess toxic, allergic and even carcinogenic properties. Along with growing concerns about sustainability and ecology, natural dyes emerge as promising alternatives. Therefore, anthocyanins, responsible for red and bluish colours in most fruit and vegetables are investigated, as they are often also abundantly available in fruit and vegetable waste, e.g. grape and berry pomace. However, these dyes have a couple of shortcomings compared to their synthetic analogues in terms of stability and affinity for substrates. For that reason, many natural dyes require dye fixatives, also called mordants. It is known that the use of metallic mordants promotes the affinity, but these do not really fit in a ‘green’ story on natural dyes. Therefore, the goal of this presentation is to show the potential of biomordants, which are selected according to the possible interactions they could undergo with the dye molecule such as hydrogen bonds, ionic bonds and π-π interactions. In order to tackle these issues, firstly, the dyeing procedures and parameters were optimized for cotton dyeing. The selection of mordants consists of tin and aluminium as reference metallic mordants and several biomordants: tannic acid, sodium alginate, β-cyclodextrin, oxalic acid, gallic acid and caffeic acid. The effect of the (bio)mordant was monitored by infrared, spectrophotometric measurements and standard ISO wash and light tests. To endorse the experimental side of this study, the aforementioned intermolecular interactions were also modelled by means of DFT calculations. Hereby, static calculations were carried out for metallic mordants and oxalic acid while molecular dynamics was applied to investigate the interaction between tannic acid and the dye molecule. This theoretical approach confirmed the experimental part: the coordination complex based on tin results into the lowest complexation energy while intermolecular interactions with other mordants are too weak to show sufficient affinity towards the cotton molecules. This combined theoretical and experimental work has characterized the boundaries of anthocyanins as a natural dye for cellulose-based materials in long term applications that undergo harsh conditions. This presentation also shows that the results from DFT calculations are useful into the future screening of biomordants.