Experimental and theoretical UV/Vis-IR-THz spectroscopies for diagnostic studies of ancient paper

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Keywords: ancient paper, degradation, UV-Vis spectroscopy, vibrational spectroscopy, density-functional-theory

During the centuries paper has been the most widely used writing support. Hence, paper degradation is a major issue for cultural heritage conservation. The main component of paper is cellulose, one of the most abundant biomaterials on Earth. Cellulose oxidation is mainly responsible for the yellowing of the ancient samples, through the formation of optically active oxidized functional groups (chromophores). This results in severe chromatic deterioration of works of art on paper. In order to investigate the yellowing of ancient paper, we applied several spectroscopic techniques (UV/Vis-IR-THz) interpreted by ab-initio theoretical computational simulations based on Density Functional theory (DFT) and Time-Dependent DFT (TDDFT) methods [1-4].

In this talk, we will illustrate our experimental and theoretical approach to the study of ancient work of art on paper. In particular, we will show how absorption spectra of cellulose fibers can be obtained from experimental UV/Vis reflectance spectra of ancient paper samples by using an improved version of the Kubelka-Munk theory suitable for strongly absorbing media. Then information on the kind and concentration of oxidized groups in cellulose is obtained by comparison with theoretical UV/Vis spectra calculated on oxidized cellulose models.

This procedure, based on experimental and theoretical UV/Vis spectroscopy, is particularly promising since it uses non-invasive and non-destructive measurements, which can be performed in-situ, allowing diagnostic analysis of delicate paper artifacts and the monitoring of their restoration interventions. Finally, we will present our results obtained in the study of precious works of art on paper, in particular on the state of degradation of the Leonardo Da Vinci's famous self-portrait.

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