

Combining Surface-Enhanced Raman spectroscopy and DFT calculations for the analysis of dyes

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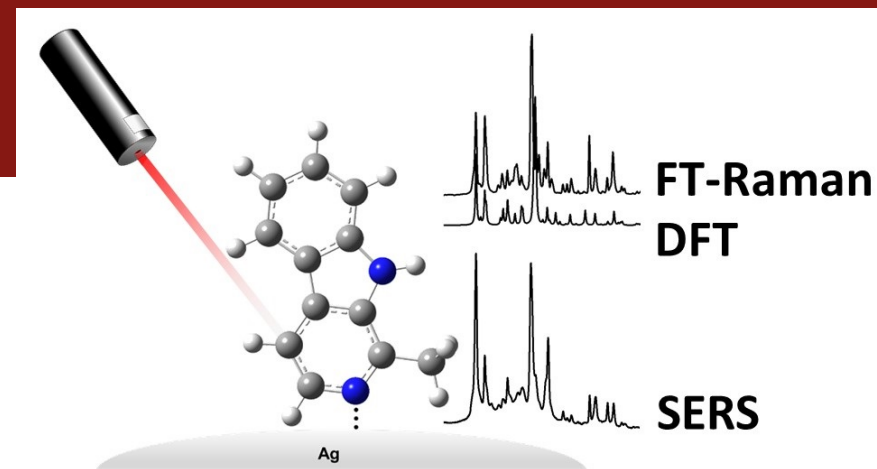
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Dr. Maria Vega Cañamares is Tenured Scientist at the Institute of the Structure of Matter of the Spanish National Research Council (CSIC) since 2012. She got her Ph.D. in Chemistry at the Universidad Complutense de Madrid. Her doctoral research focused on the application of Surface-Enhanced Raman Spectroscopy (SERS) to the study of natural dyes. Maria Vega was awarded an Andrew W. Mellon Fellowship in Conservation at the Metropolitan Museum of Art in New York, where she specialized on the analysis of

dyed textiles by SERS. She held a second postdoctoral position at the City College of New York where she worked on the SERS analysis of synthetic dyes. During her career she has combined experimental work with the use of computational chemistry methods like Density Functional Theory (DFT). She uses DFT to simulate the vibrational spectrum of dyes to aid in the assignment of the vibrational normal modes. She leads the “Raman and IR spectroscopy: Application in Art and Archaeology” research line at the CSIC Archaeology Network.



Comparison of the experimental FT-Raman and the DFT calculated Raman spectrum of an alkaloid molecule together with the SERS spectrum and the proposed interaction of the molecule on Ag nanoparticles.