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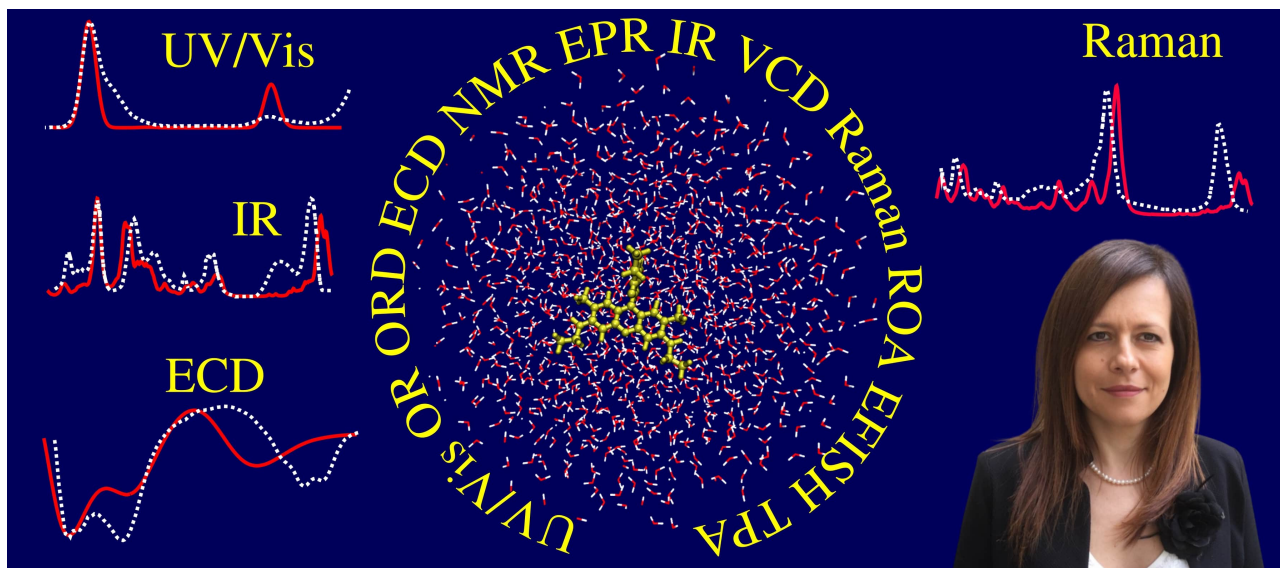Online (URL in E-Mail)

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Computational Spectroscopy of Solvated Systems

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The spectral response of molecular probes strongly depends on the surrounding environment. A successful approach to computational spectroscopy of systems in the condensed phase consists of resorting to focused models, where the focus is on a specific portion of the system, which is described at the Quantum Mechanical (QM) level, whereas the remaining portion is treated classically, through ad-hoc Molecular Mechanics (MM) force-fields [1]. Polarizable QM/MM approaches, where the mutual polarization between QM and MM layers is considered [2,3], are particularly successful in modelling spectral properties of molecular systems embedded in complex external environments [2,3].

I will discuss the most recent developments of the fully polarizable QM/FQ(Fμ) approach to computational spectroscopy [2-4], by resorting to pilot applications [5-10], which highlight the method's potentialities.

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