

## TOWARD COMPUTATIONAL SPECTROSCOPY STUDIES FOR LARGE MOLECULAR SYSTEMS

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Integrated computational approaches built on quantum mechanical (QM) methods combined with time-independent schemes to account for nuclear motion effects are applied to the spectroscopic investigation of molecular systems, from large biomolecules to hybrid supra-molecular systems. Within the time-independent approaches, vibrational spectra are computed including anharmonicities through perturbative corrections while UV-vis line-shapes are simulated accounting for the vibrational structure; in both cases, the environmental effects are taken into account by explicit or continuum models. Extension to larger systems relies on reduced dimensionality approaches and effective schemes to select transitions of interest, available for both vibrational and vibronic spectra. Such procedures are exploited to simulate IR and UV-vis spectra leading in all cases to good agreement with experimental observations and allowing to dissect different effects underlying spectral phenomena, finally, paving a feasible route toward the state-of-the-art computational spectroscopy studies, even for relatively large molecular systems [1,2].

1. V. Barone, A. Baiardi, M. Biczysko, J. Bloino, C. Cappelli, F. Lipparini *Phys. Chem. Chem. Phys.*, 14, 12404, 2012
2. V. Barone, M. Biczysko, J. Bloino, M. Borkowska-Panek, I. Carnimeo, P. Panek, *Int. J. Quantum Chem.* 112, 2185, 2012