TOWARD COMPUTATIONAL SPECTROSCOPY STUDIES FOR LARGE MOLECULAR SYSTEMS

MALGORZATA BICZYSKO, *Center for Nanotechnology Innovation@NEST, Istituto Italiano di Tecnologia, Piazza San Silvestro 12, I-56127 Pisa, Italy*; JULIEN BLOINO, *Consiglio Nazionale delle Ricerche, Istituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), UOS di Pisa, Area della Ricerca CNR, Via G. Moruzzi 1, I-56124 Pisa, Italy*; VINCENZO BARONE, *Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126 Pisa, Italy*.

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 lineshapes 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