3D structures of (Ac-Phe-OMe)1,2 peptides by DFT-MD : Graph Theory for the assignment of far-IR gas phase IR-UV ion dip spectra

Daria Ruth Galimberti
Institute for Molecules and Materials (IMM), Radboud University, Nijmegen (The Netherlands)
daria.galimberti@ru.nl

I will present a newly developed method [1] for the assignment of (anharmonic) vibrational modes from MD simulations, based on Graph Theory coupled to APT weighted-internal coordinates velocities DOS spectra [2]. The strategy is organized over two steps: the first step consists in reconstructing the theoretical IR spectrum in terms of the contributions of the APT weighted-internal coordinates velocities [2]; the second step consists in applying Graph Theory algorithms to transform these data into graphs where the vertices are the internal coordinates that participate to the modes (self-terms) and the edges represent the internal coordinates cross-terms.

The graphs hence obtained show the atomic motions that participate to each given vibrational mode, whether the mode is localized or delocalized (i.e., a collective motion), how many coupled motions participate to the mode(s), together with the percentage of participation of each of the contributor to the mode(s). Similarities between graphs can be obtained, providing similarities in between vibrational modes. This is especially useful when assigning the vibrational spectra of dimers, providing the similarities/disimilarities in the modes in going from the monomer to the dimer. As a test case I will present the study of the 3D structures of $(Ac\text{-}Phe\text{-}OMe)_{1,2}$ peptides by combining gas phase IR-UV ion dip spectroscopy experiments, using the far-IR/THz signatures (100-800 cm^{-1}), with DFT-based molecular dynamics simulations.

[1] D.R. Galimberti et al. Faraday Discuss., 2019,217, 67-97
[2] D. R. Galimberti et al-J. Chem. Theor. Comput., 13(8), 3802-3813, 2017