QUANTUM-MECHANICAL PROTOCOLS FOR DECODING LIGHT–MATTER INTERACTIONS

Malgorzata Biczysko

Faculty of Chemistry, University of Wroclaw, Wroclaw, Poland
malgorzata.biczysko@uwr.edu.pl

Molecular systems of increasing size and complexity from small prebiotic molecules of astrochemical interest [1,2], medium size chromophores important for technology applications [3] to larger bio-molecules such as proteins [4,5] are nowadays studied by broad range of experimental techniques, involving different parts of electromagnetic spectrum [6], as depicted in Figure 1. However, it is seldom straightforward to link the rich experimental data to the desired information on the specific structure and properties of complex molecular systems.

I will discuss status and perspective of the project aimed at development, validation and application of QM based computational protocols supporting to decode and analyze experimental data based on light-matter interaction.

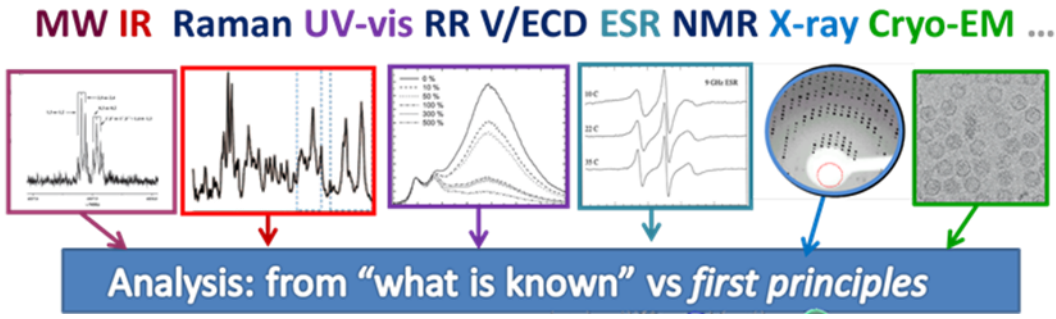

Figure 1. First principles support for experiments.

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