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UCZELNIA BADAWCZA
INICJATYWA DOSKONAŁOŚCI

Computational protocols for molecular structure and spectroscopy

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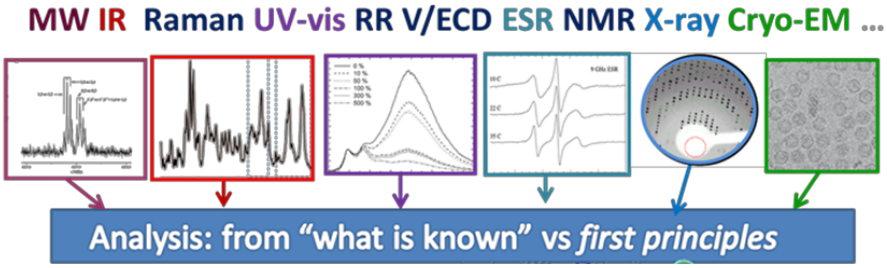
Molecular systems of increasing size and complexity from small prebiotic molecules of astrochemical interest [1,2], medium size chromophores important for technology applications [3] to larger bio-molecules such as proteins [4,5] are nowadays studied by broad range of experimental techniques, involving 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.



Rysunek 1: QM support for experiment

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[2] X. Yanting, M. Biczysko, "Toward the identification of cyano-astroCOMs via vibrational features: benzonitrile as a test case", *Front. Chem.* 12, 1439194 (2024).

[3] R. Zubatyuk, M. Biczysko, K. Ranasinghe, N. W. Moriarty, H. Gokcan, H. Kruse, B. K. Poon, P. D. Adams, M. P. Waller, A. E. Roitberg, O, Isayev, P. V. Afonine "AQuaRef: machine learning accelerated quantum refinement of protein structures", **Nat. Commun.** 16, 9224 (2025).

[4] Y. Liu, M. Biczysko, N. W. Moriarty, „A radical approach to radicals", *Acta Cryst.* D78, 43-51 (2022).

[5] V. Barone, S. Alessandrini, M. Biczysko, J. R. Cheeseman, D. C. Clary, A. B. McCoy, R. DiRisio, F. Neese, M. Melosso, C. Puzzarini, "Computational molecular spectroscopy", *Nat. Rev. Methods Primers* 1, 38 (2021).