

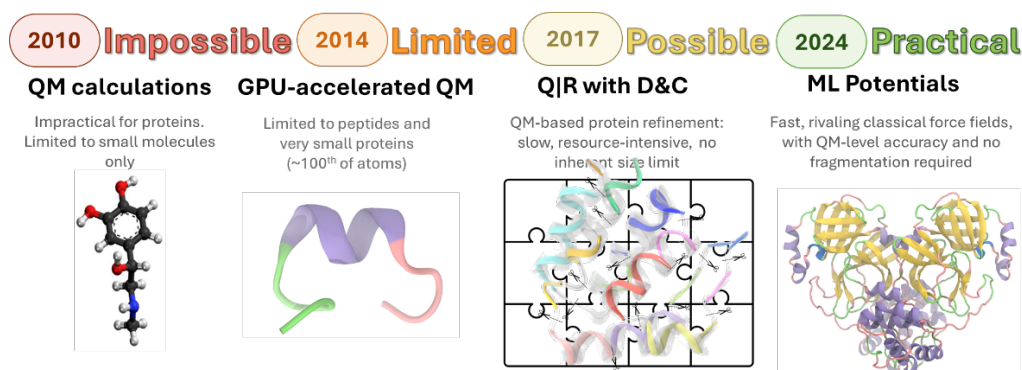
QM- and AI-based Approaches to the Structure and Spectroscopy of Biological Macromolecules

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Protein structures and their physicochemical properties are essential for understanding biological function and improving drug–protein interactions. Most structures in the Protein Data Bank (PDB) [1] have been determined by X-ray crystallography and cryo-electron microscopy, while recent advances in structure prediction [2] support but do not replace experimental studies [3].

Spectroscopic techniques provide complementary insight into protein dynamics and environmental effects, yet structural and spectroscopic data are often analyzed separately. Quantum chemistry (QM) computations establish a physically grounded link between molecular structure and spectroscopic observables, enabling direct comparison with experiment. This is particularly important for proteins and protein–ligand systems, where local interactions and spatial confinement can significantly affect structural and spectral properties. In this talk, I will present a project developing integrated computational tools that use QM and AI-based approaches to improve structural consistency and advance understanding of protein properties through systematic integration of experimental data [4-10].



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