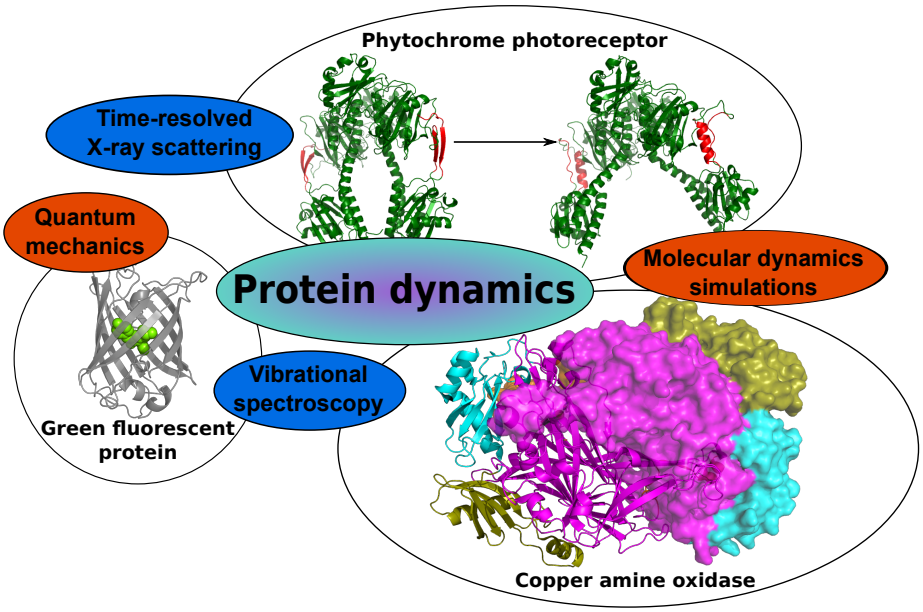
Combining theoretical and experimental methods to study protein dynamics

Proteins fulfill a wealth of tasks in living organisms. Understanding their function on a molecular level is of fundamental interest in life sciences with applications in drug design, crop sciences and energy production. While there are already well-established methods available to determine protein structures, methods to investigate protein dynamics with atomic resolution are still scarce and mostly have to be tailored to the respective protein system.

In this talk I will describe protein dynamics studies of different systems and show how theoretical methods can help in designing and analyzing these experiments. The size of the proteins spans a range from 7000 to 20000 atoms starting with green fluorescent protein[1] turning to the phytochrome photoreceptor with around 10000 atoms[2, 3] and finally giving an outlook to a copper amine oxidase[4] which is the focus of future studies.



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