

SFB  
1078



Protonation Dynamics  
in Protein Function

Mon, November 09,  
2020

15:15 – 16:15

Freie Universität Berlin

via WebEx

## ➤ Colloquium

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### Tailored multi-level vibrational theory - A computational magnifying glass for marker bands in vibrational spectra -

Vibrational spectra are highly sensitive to structural changes while offering a high time resolution. Therefore, vibrational spectroscopy is an excellent tool to follow reactions as well as conformational changes in biomolecular systems. Already for small oligopeptides, however, the interpretation of full spectra is highly challenging. Fortunately, we are often only interested in certain bands and how they evolve during a process. Experimentally, difference spectroscopy offers an excellent magnifying glass to resolve such changes. This allows, for instance, to follow reactions of protein cofactors in which a handful of hydrogen bonds are affected and to single out their effect from that of the many hydrogen bonds presents in a protein. Still, the structure-spectra mapping is inherently difficult and benefits tremendously from computational assistance. The available computational methods are, however, highly challenged by such applications, as their computational effort scales steeply with system size. This holds especially true when highly anharmonic vibrations, such as hydrogen-bonding vibrations, are of interest.

Similar to difference spectroscopy, multi-level computational approaches allow to focus the computational effort on selected parts of the system. By this, conclusive results can be obtained with much reduced computational effort. In the above example, one could, e.g., treat the vibrational degrees of freedom associated with the hydrogen-bond stretches in an accurate, anharmonic manner, while pay less attention to the other degrees of freedom.

In this talk, I will outline the basic ideas and benefits of multi-scale methods, which are well established for the electronic problem. I will further present our initial work on transferring this concept systematically to the field of vibrational wave functions. For future application of those methods to oligopeptides and proteins, several aspects need to be considered: This includes the choice of vibrational coordinates to span the vibrational space, electronic structure fragmentation and multi-level methods for the generation of the underlying potential energy surface as well as reduced and divided vibrational spaces. The latter will be shown for the harmonic treatment of amide bands of a small peptide as well as for examples of vibrationally resolved UV/Vis emission spectra of organic fluorescent biomarkers. With this in mind, I will outline a way ahead with a focus on the application of such methods to biomolecular problems, such as the calculation of difference infrared spectra following a protein reaction based on a reorganization of a few hydrogen bonds.

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