**International Graduate Research Training Group 1524**

**Self-Assembled Soft-Matter Nanostructures at Interfaces**

**– Colloquium –**

**Tuesday, February 12th, 2013, 17.15 h(!):**

**Technische Universität Berlin**
**PC building, room PC 203**
**Strasse des 17. Juni 135, 10623 Berlin**

## Prof. Dr. Steven Boxer

Stanford University, Stanford, California, U.S.A.

# „Electrostatics in proteins using vibrational Stark spectroscopy“

Electrostatic interactions impact every aspect of the structure and function of proteins, nucleic acids, and membranes. The transition states for many enzyme-catalyzed reactions involve a change in the distribution of charge relative to the starting material and/or products, and the selective stabilization of charge-separated transition states may be essential for catalysis. The magnitudes of the electric fields in proteins and the variations in these fields at different sites are predicted to be enormous, but it is a challenge to obtain quantitative experimental information on these fields. We have developed vibrational Stark effect (VSE) spectroscopy to probe electrostatics and dynamics in organized systems, in particular in proteins where they can report on functionally important electric fields. The strategy involves deploying site-specific vibrational probes (-C≡N, -C-D, -C=O and –C-F) whose sensitivity to an electric field is measured in a calibrated external electric field by VSE spectroscopy. This gives the magnitude of the vibrational frequency shift associated with an electric field change in a protein, e.g. by making a mutation, changing pH, ligand binding, etc., projected along the bond axis, which is typically determined by x-ray crystallography. This concept can also be used to estimate the electrostatic contribution to non-covalent interactions such as X-H••π interactions that stabilize protein structures. Recent results in which we attempt to calibrate the absolute magnitude of the field will be presented. This requires a substantial development of simulation methods in parallel with experiments. By fully understanding the origins of these effects, they can be applied to obtain information on functionally relevant electric fields at the active site of enzymes. In a first example, we are able to directly correlate the field sensed at the bond involved in enzymatic catalysis and the rate of the reaction it catalyzes, including perturbations to this rate in a series of mutant. This approach provides experimental benchmarks for high-level simulations that have suggested a critical role for electric fields and electric field gradients in biological function.

We cordially invite everybody who is interested.

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