SFB 1078

Protonation Dynamics in Protein Function

Mon, **Jan. 11**, 2016

16:15 – 18:30

Freie Universität Berlin
Physics Department
Lecture Hall B

(Arnimallee 14, 14195 Berlin-Dahlem)

Colloquium

Dr. Syma Khalid – University of Southampton, UK

Capturing the Complexity of Bacterial Membrane-Protein Interactions by Molecular Dynamics Simulations

Gram-negative bacteria such as *E.coli* are typically regarded as "simple" model organisms, yet their cell envelopes are surprisingly complex. To study the influence of the bacterial membrane on the dynamics of outer membrane proteins (OMPs), antimicrobial peptides and other nanomaterials, S. Khalid and her group have created a virtual *E.coli* outer membrane using atomistic & coarse-grain approaches. She will present some of their successes and also current limitations and plans for the future.

Dr. Nicholas Cox – MPI for Chemical Energy Conversion, Mühlheim, Germany

Spin state as a marker for the structural evolution of Nature's water splitting catalyst

In a recent report the structure of nature's water splitting catalyst - a Mn_4O_5Ca cofactor - in its final metastable catalytic state (S_3) was resolved [Cox *et al.* (2014) *Science* 345:804]. Its structure is similar to that seen by X-ray crystallography, but requires the coordination of an additional water molecule to the cluster, as a hydroxide, rendering all Mn ions six coordinate. Interestingly the precursor (S_2) state exists in two isoenergetic but structurally distinct conformations [Pantazis *et al.* (2012) *Angew. Chem. Int. Ed.* 51:9935]. N. Cox will describe how the ability of the Mn_4O_5Ca cofactor to adopt two distinct structural and spin-state forms in the S_2 state is critical for water binding in the S_3 state, allowing spin state crossing from the inactive, low-spin configuration of the catalyst to the activated, high-spin configuration.

Coffee and tea are ready at 16:00 and during the break from 17:10 – 17:30.

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