KN7 ***Listeria Monocytogenes* Lmo0818 – Exploring a putative Ca^{2+}-ATPase, to understand Calcium ion specificity**. Kim Langmach Hein[a], J. Preben Morth[a]
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The ongoing progress in the Ca^{2+}-ATPase field and the general field of P-type ATPases, reveals a clear goal for membrane structural biology: We need many structures of the same protein stabilised in different distinct states to fully understand how the individual protein function. Questions with regards to substrate recognition, selectivity and transport can thus be addressed with stronger confidence. These questions are still not fully understood despite the fact that more than 9 different states of the Ca^{2+}-ATPase are available in the Protein databank [1].

This project focus on calcium homeostasis in the opportunistic pathogenic bacteria *Listeria monocytogenes*. Genomic analysis of *L. monocytogenes* identifies two P-type ATPases with putative selectivity for Calcium transport (Lmo0841 and Lmo0818). Lmo0841 was recently confirmed as a Ca^{2+} -ATPase, able to transport a single Calcium ion per hydrolyzed ATP the *L. monocytogenes* Ca^{2+} -ATPase was consequently named LMCA1 [2]

Sequence analysis and homology modeling strongly suggest that Lmo818 is a Ca^{2+}ATPase with high similarity to the plasma membrane ATPases (PMCA), a type IIb P-type ATPase from higher eukaryotes. There is no X-ray structures of any PMCA's determined , they are known to be less stabile in comparison with the sarco(endo)plasmic reticulum Ca^{2+} -ATPases (SERCA) and also often require additional soluble factors to function, like the necessity of Calmodulin to the PMCA [3]. We have determined the structure to 2.8 Å resolution initial structural comparison indicate a similar fold to SERCA, however with significantly reduced loop regions. A comparative bioinformatics study will be presented based on Lmo0818 that reveal how a divalent ion could be recognized and selectively transported in these prokaryotic membrane systems as compared to ion recognition found in the SERCA and the Na^+,K^+ -ATPase [4][5].

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KN8 **Time Resolved Crystallographic Processes in Molecular Systems.** Simone Techert, *IFG Structural Dynamics of (bio)chemical Systems, Max Planck Institute for Biophysical Chemistry, Goettingen, Germany*
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Molecular crystals have the potential to be used i.e. in molecular electronics, optoelec-tronics, as molecular switches, in sensor technology or as pharmaceuticals. In order to optimize their performances, ideally the knowledge of their time-dependent structure - function relation is required. Characteristic for all chemical reactions in molecular solids are bond breaking and bond making processes. Our vision is to optimize these structures towards specific product states by a clever combination of chemical site-specificity, self-assembly and state-selectivity which can be "tuned" from orbital control through the structure of the local environment and selective excitation schemes (heat / optical pulses) to bulk structural changes – or to say it in other words – from the simple to the complex. We would like to understand - what are the driving forces of environment and light for tuning chemistry?

In the present contribution we will give an overview on our strategy utilizing the pulsed characteristics of x-ray sources, in particular synchrotrons and free electron lasers, to gain such information. On the x-ray methodological side, molecular crystals form the ideal matrix to proof the capabilities of ultrafast radiation generated with Free Electron Lasers (FLASH at DESY or LCLS at SLAC). In the current contribution we will present our studies on the possibility to collect the "molecular movie" with spatial resolution down to electron density distribution on femtosecond time scales. Last are the typical time scales of atomic and charge movements (in particular within the Born Oppenheimer limit). Common for all time-resolved x-ray experiments is the applied pump / probe scheme, where an optical pump-laser initiates a reaction whose structural time evolution is then investigated by x-ray probe pulses at various time delays. The x-ray photon-in/photon-out techniques are based on diffraction or spectroscopic techniques like near edge spectroscopy or x-ray emission spectroscopy. Meanwhile x-ray spectroscopic techniques probe the local environment around specific atoms in a molecule such as orbitals, crystallographic experiments (monochromatic or Laue) reveal the structure of the bulk of periodic systems. (Time-resolved diffuse x-ray scattering experiments give information about the structure of liquids.)

Finally, we will present our efforts in systematizing the characteristic structural changes in molecular systems during chemical reactions to some kind of "periodic table" of structural dynamics allowing to predict reaction properties in chemistry from a time-dependent structural point of view.

Keywords: time-resolved crystallography, free electron laser research, molecular crystals