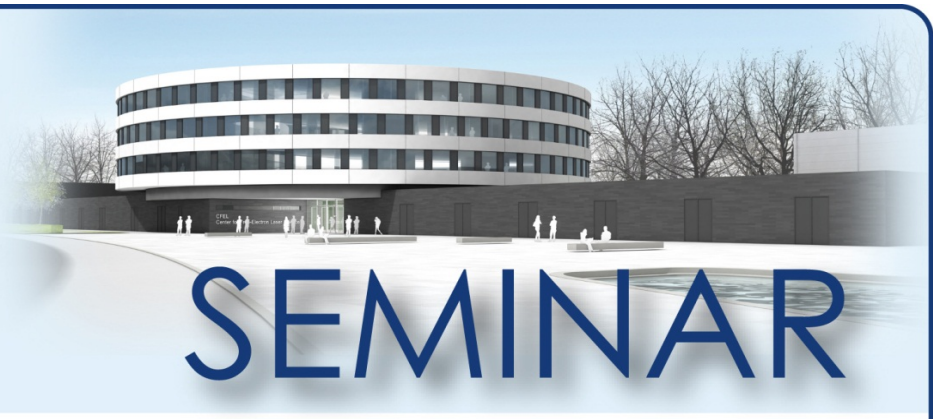
CFEL SCIENCE



SEMINAR

14th February 2013 - 10:00

Building 99, Seminar Room II (EG)

Anouk Rijs

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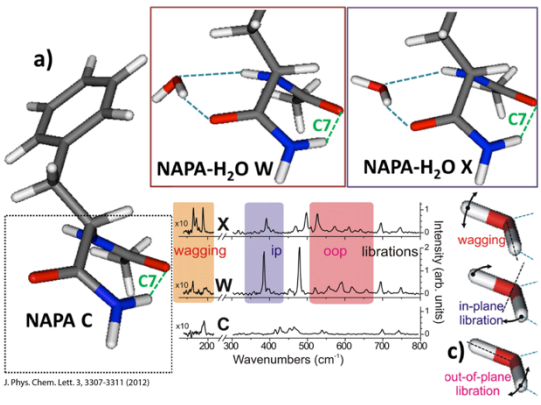
Flexibility and rigidity in peptides probed by gas-phase mid & far-IR Spectroscopy

In nature, proteins combine soft and hard matter properties: Stability requires stiffness, whereas function requires motion and a degree of floppiness. The step of forming a structural motif leads to a considerable stiffening of a peptide, blue-shifting of in particular the soft vibrational modes, causing a substantial reduction in the vibrational state density. Experimental mid- and far-IR signatures will reveal such effects and provide further understanding of backbone motion and flexibility versus rigidity.

We will focus on three motifs often found in proteins by using peptide mimics. These motifs are (i) gamma turns, (ii) helices, and (iii) interactions with water molecules mimicking the hydrate interactions. To investigate the IR signature of the peptide motifs, we employ the powerful mid and far-IR free electron lasers available in the new FELIX facility Nijmegen. Low-frequency vibrations in peptides typically involve the collective motion of the entire backbone of the molecule, in contrast to high-frequency modes which are typically localized on one or a few chemical bonds. The low-frequency modes are therefore particularly sensitive to the overall structural motif, such as the well-known helical or sheet-like motifs in proteins, while the mid-IR reveals intra-molecular interactions. The experimental results will be interpreted in combination with quantum-chemical calculations and molecular dynamics simulations.



Host: Melanie Schnell - CFEL Molecular Physics seminar