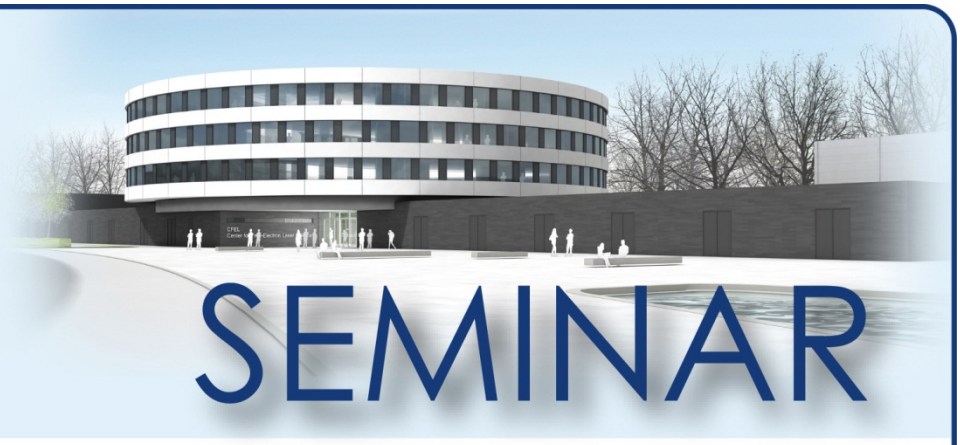
CFEL SCIENCE



SEMINAR

21st February 2012 - 14:15
FLASH HALL (28c) - Seminar Room

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Dynamics of processes at surfaces and interfaces studied from first principles

Processes at surfaces and interfaces such as catalytic reactions, corrosion or crystal growth are technologically of strong relevance. They are, however, also interesting from a fundamental point of view since this research field is at the borderline between solid-state physics and chemistry. Due to the increase in computer power and the development of efficient algorithms it has become possible to perform ab initio molecular dynamics (AIMD) simulations of processes at interfaces in which the forces necessary to solve the equations of motion are obtained from first principles "on the fly". This allows to elucidate the dynamics of multi-atomic molecules interacting with complex surface and interface structures.

In this contribution, I will present recent AIMD studies of the interaction of molecules with precovered surfaces [1]. Furthermore, catalytic processes involving concerted reaction mechanisms in the methanol synthesis will be discussed. Finally, atomistic structures and processes at solid-liquid interfaces will be addressed [2] which are relevant, e.g., in the electrochemical energy conversion and storage.

[1] A. Groß, J. Chem. Phys. 135, 174707 (2011).
[2] S. Schnur and A. Groß, New J. Phys. 11,125003 (2009); Catal. Today 165, 129-137 (2011).

Host: Martina Dell'Angela & Wilfried Wurth, UHH-ASG