Controlled chemistry

Doctoral thesis project

CFEL SCIENCE
Controlled Molecule Imaging

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The Controlled Molecule Imaging group at the Center for Free-Electron Laser Science at DESY and Universität Hamburg performs novel experiments on the control and imaging of gas-phase molecules and their ultrafast dynamics with applications in fundamental physics, chemistry and structural biology.

We develop new experimental approaches to cool and control complex molecules, such as spatial separation of individual molecular species, alignment and orientation of molecules in space, and the creation of well-defined molecular wavepackets. We image molecular structures and dynamics — recording movies of molecules at work — using ion and electron imaging as well as coherent diffractive imaging techniques with x-rays and electrons. This work is accompanied by sophisticated data analysis, computational modeling, and *ab initio* theory developments.

Structure-function relationship in “cold” chemical reactions

We are investigating the structure-function relationship of conformer-selected complex molecules. In collaboration with the Willitsch group in Basel we have performed pioneering benchmark experiments to investigate structure-dependent chemical reactivities (see reference below). These experiments are now extended to the investigation of conformer-separated molecule-molecule reactions.

In this project the candidate will extend our benchmark studies to the investigation of conformer specific reactivity studies of complex chemical reactions, such as cycloadditions (Diels-Alder reactions) and other textbook examples, in order disentangle the microscopic details. This involves the experimental verification of relevant molecular properties in deflection and spectroscopy experiments, and the measurement of conformer specific reactivities. Moreover, the detailed analysis requires programming, simulations of the deflection process, and quantum-chemistry calculations. This project will involve repeated travel to our collaborators at the University of Basel, Switzerland.

A successful candidate will have a strong background in physical chemistry, molecular physics, or a related field. Experience with molecular beams, high-vacuum equipment, short-pulse lasers or quantum-chemistry codes is a plus.

Science, **342**, 98–101 (2013) – http://dx.doi.org/10.1126/science.1242271
Phys. Rev. Lett. **100**, 133003 (2008) – http://dx.doi.org/10.1103/PhysRevLett.100.133003
Angew. Chem. Int. Ed. **48**, 4900 (2009) – http://dx.doi.org/10.1002/anie.200900755

CMI offers unique research opportunities in an interesting, open, international team and with first-class experimental and computational facilities. Our group is embedded in the Center for Free-Electron-Laser Science, Deutsches Elektronen-Synchrotron DESY, Universität Hamburg, and the Hamburg Center for Ultrafast Imaging.

https://www.controlled-molecule-imaging.org

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