

NEWSLETTER

CUI – Graduate School

No.9, August 2015

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Editorial

Our cluster is approaching its third birthday, meaning that we have just surpassed half of its (first) funding period. In this time CUI members have obtained an impressive number of recognitions and several major scientific objectives have been attained. The numbers speak for themselves: Since November 2012, 18 CUI members have received an award and 4 of them were young researchers. Furthermore, since then CUI has lead to more than 120 papers and of them 11 were published in the Nature family, 6 in Science and 15 in Physical Review Letters. Last but not least, the training of our PhD students is also working extremely well as they have organised their third winter school. All this does not only demonstrate the quality of the research carried out within CUI, but it makes us very confident for the future.

Antonio Negretti and Peter Schmelcher

Course programme

The course programme of the next winter term has the CUI main lecture *When laser physics meets life science: A trial for a basic introduction* by Dr. Markus Perbandt and Dr. Guoqing Chang.

The detailed course programme with the time schedule and abstracts can be downloaded at the webpage of graduate school of CUI.

Winter school

The PhD students are actively working on the organisation of the next winter school, which will take place from Monday February 15 to Friday February 19, 2015. The event will be organised in the Hotel Schwarzwaldgasthof Rößle in Todtmoos-Strick in the south of Germany, a quite place immersed in the Nature.

As usual the organisation committee has prepared a structured lecture programme covering all the research areas of our cluster of excellence CUI.

Research highlights

The CUI scientists Dr. M. A. Schroer and Dr. F. Lehmkuhler of the group led by Prof. G. Grübel together with their colleagues have introduced a new technique, nano-beam X-ray cross-correlation microscopy (XCCM), which allows the study of the local orientational order in matter with high spatial resolution. In particular, it permits studying systems showing only short-range order, such as glassy

systems, using a nanofocus X-ray beam of $400 \times 400 \text{ nm}^2$ provided by the GINIX instrument at the beamline P10 of PETRA III. They demonstrated the potential of XCCM by studying densely-packed thin films made out of dried binary mixtures of spherical silica particles. For these films, the structure and orientational order were determined with high spatial resolution. The work was published in *Soft Matter* 11, 5465 (2015).

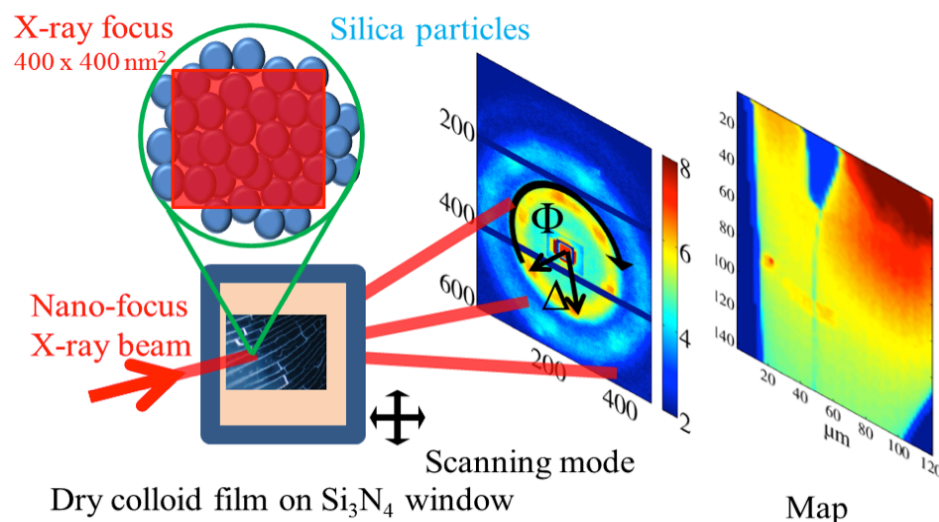


Fig. 1: Schematic setup of the XCCM experiment.

Personalia

Prof. R. J. Dwayne Miller (Max Planck Institute for the Structure and Dynamics of Matter) has been awarded from the Canadian Institute for Advanced Research with the project "Molecular Architecture of Life". His project was one of the top four supported projects of 260 proposals from all over the world and fields including humanities and law.

Prof. Alexander Lichtenstein (Institut für Theoretische Physik) has received from the Czech Academy of Science the Ernst Mach-Medal 2015 for his outstanding achievements in Physics.

The Editorial Board of the New Journal of Physics has appointed Prof. Jochen Küpper (Center for Free-Electron Laser Science) as "outstanding referee".

The CUI postdoctoral researcher Dr. Philipp Wessels (Zentrum für Optische Quantentechnologien) has received a second prize of the Deutscher Studienpreis awarded by the Körber Foundation for his dissertation on "Live images from the nanocosmos – Ultrafast magnetization processes of smallest structures in slow motion".

Congratulations to the award winners!



R. J. Dwayne Miller



Alexander Lichtenstein



Jochen Küpper



Philipp Wessels

The CUI PhD student S. Zinn and her collaborators in the group led by Dr. M. Schnell of the Max Planck Institute for the Structure and Dynamics of Matter has recently investigated the structural properties of the conformers of ibuprofen in the gas phase. The drugs based on ibuprofen are well known in our society. Its pain-relieving properties arise from its ability to physically block the active site of an enzyme. The ability of the molecules to adjust their structure by different arrangements of individual side chains can be a key in such a molecule-specific blocking process. This makes the structural and conformational properties of pharmaceutically relevant molecules such as ibuprofen highly interesting.

Ms. Zinn and coworkers have performed a conformer-selective high-resolution rotational spectroscopy study of ibuprofen in order to elucidate its structural and conformational flexibility. The precise molecular parameters determined in this high-resolution molecular

spectroscopy study are for example useful for benchmarking quantum-chemical calculations. Interesting insight about the conformational landscape could be gained. The researchers could identify four low-energy conformers that only differ in the orientation of the isobutyl group, i.e., one of the branched side chains of ibuprofen, with respect to the rest of the molecule. A scheme of the experimental approach and the obtained broadband rotational spectrum illustrating the molecular fingerprint arising from the four ibuprofen conformers is displayed in Fig. 2. In-

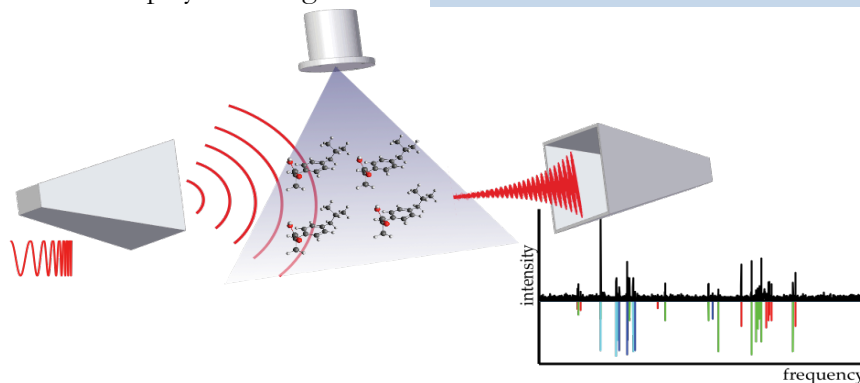


Fig. 2: (Left) Sketch of the measurement scheme used to determine the structural and conformational flexibility of ibuprofen. (Right) The four conformers of ibuprofen are identified by their broadband rotational spectra. The black line corresponds to the experiment, while the coloured vertical lines are fits to the rigid-rotor Hamiltonians. The four colours correspond to the four conformers of ibuprofen.

terestingly, the molecular subgroup that is known to bind to the active site of an enzyme, i.e., the propionic acid group, favours a stable arrangement. Giving these findings, one can speculate that the flexibility of the isobutyl side chain is required for approaching the reaction site, while the stable propionic acid group will then selectively bind. The work has been published in Phys. Chem. Chem. Phys. 17, 4538 (2015).

Mildred Dresselhaus Guest Professors 2015

We warmly welcome Prof. Elspeth Garman (Oxford University) and Dr. Liesbeth Janssen (Heinrich-Heine Universität Düsseldorf) as CUI guest professors.

We wish them a very productive and successful work during their stays at CUI.

Important dates in 2015-16

We remind you that at November 7 the Night of Knowledge/Open Day and in November 11-12 the next CUI International Symposium in conjunction with the Hamburg Prize for Theoretical Physics will take place. Just afterwards we shall have our Annual Meeting (November 13-15) at the Baltic Sea, Hotel Hohe Wacht in Hohwacht. Finally, the next graduate days of CUI will take place in March 14-17, 2016.

Please, mark these important dates in your agenda!

You are welcome to: ... send us suggestions of topics which you would like to be mentioned in the next newsletter (anegrett@physnet.uni-hamburg.de).