Tuesday, 01.09.2015, Room EI 3

Time	ID	Combined Session *Chair: Stéphane Goyette, Uni Genève*
13:30	601	**Fully Consistent Finite-Strain Landau Theory for High-Pressure Phase Transitions** *Andreas Tröster* *Institute of Material Chemistry, Vienna University of Technology, Getreidemarkt 9, AT-1060 Vienna* A new generalization of the Landau theory of structural phase transitions allows to systematically handle the large geometrical and physical nonlinearities at high pressure for the first time [PRX 4, 031010 (2014)]. Central to our approach is the pressure dependence of elastic constants, which may be taken from experiment or DFT. The practical feasibility, precision and predictive power of our theory is illustrated by an accurate description of recent high-quality experimental data for the high-pressure cubic-tetragonal phase transition in strontium titanate, including the prediction of a number of elastic transition anomalies yet to be confirmed by experiment.
13:45	602	**Modeling the Absorption of Microwaves in Multicomponent Rock** *Ronald Meisels [1], Michael Toifl [2], Philipp Hartlieb [3], Friedemar Kuchar [1], Thomas Antretter [2]* *[1] Institute of Physics, Montanuniversität, Franz Josef Str 18, AT-8700 Leoben* *[2] Institute of Mechanics, Montanuniversität, Franz Josef Str 18, AT-8700 Leoben* *[3] Chair of Mining Engineering and Mineral Economics, Montanuniversität, Franz Josef Str 18, AT-8700 Leoben* Of the energy needed to crush rocks only a small part is actually spent producing new surfaces. Weakening the rock structure by microwaves induced fractures could enhance the energy efficiency. In this work the propagation of these microwaves is simulated using the FDTD algorithm. A 3D model of the rock is composed of irregular polyhedra randomly assigned the different dielectric properties of the rock components, e.g. quartz (non-absorbing) and plagioclase (strongly absorbing). The calculated inhomogeneous absorption is used to determine the temperature and stress distribution. Supported by the Austrian Science Fund (FWF) project TRP284-N30.
14:00	603	**Reactions of Nitrogen Oxides With Hydrated Ions** *Christian van der Linde [1], Robert F. Höckendorf [2], O.-Petru Balaj [2], Martin K. Beyer [1]* *[1] Inst.für Ionenphysik & Angewandte Physik, Univ. Innsbruck, Technikerstr. 25/3, AT-6020 Innsbruck* *[2] Inst. für Physikal. Chemie, Christian-Albrechts-Universität zu Kiel, Olshausenstr. 40, DE-24098 Kiel* Nitrogen oxides are an important compound in tropospheric chemistry. Their reactivity with volatile organic compounds is well understood, but radical anion reaction pathways may also play a role. Free electrons are generated in the atmosphere by ionizing radiation, combining largely with oxygen and possibly carbon dioxide. Anionic water clusters like $(H_2O)n^-$, $O_2^-(H_2O)n$ or $CO_2^-(H_2O)n$ are excellent models to gain insights into their chemistry with nitrogen oxides N_xO_y. A Fourier-Transform Ion Cyclotron Mass Spectrometer, equipped with a laser vaporization ion source, is used to study these reaction systems. Kinetics and thermochemistry, applying a nanocalorimetric approach, are analyzed in detail.
14:15	604	**A bi-functional surface emitting and detecting mid-infrared device for sensing applications** *Andreas Harrer [1], Benedikt Schwarz [1], Rolf Szedlak [1], Johannes Waclawek [2], Harald Moser [2], Donald MacFarland [1], Tobias Zederbauer [1], Hermann Detz [1], Aaron Andrews [1], Werner Schrenk [1], Bernhard Lendl [2], Gottfried Strasser [1]* *[1] TU Wien, Institute for Solid State Electronics, Floragasse 7/I, AT-1040 Wien* *[2] TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, AT-1060 Wien* Mid-infrared light sources and detectors offer promising capabilities for chemical sensing of liquids and gases. Ring quantum cascade lasers (ring-QCL) exhibit a low divergence angle and modifiable far fields [1]. A distributed feedback ring-QCL and a metal photonic crystal detector were processed from

		a material designed for same frequency lasing and detection [2]. The surface emitted light from the ring-QCL is collimated, reflected by a flat mirror and focused back onto the detector. With the emission/ detection wavelength of 6.5μm gas concentrations of n-Butane and Propane were measured utilizing a single pass gas cell placed between the device and a mirror. Concentrations from 10% to 90% n-Butane in Nitrogen were detected.
14:30	**605**	**Conductance measurements of individual molecular wires** *Christophe Nacci [1], Francisco Ample [2], David Bleger [3], Stefan Hecht [3], Christian Joachim [4], Leonhard Grill [1]* *[1] University of Graz, Heinrichstrasse 28, AT-8010 Graz* *[2] IMRE, 3 Research Link, SG-117602 Singapore* *[3] Humboldt University, Brook-Taylor-Str. 2, DE-12489 Berlin* *[4] CNRS CEMES, 29 Rue Jeanne Marvig, FR-31055 Toulouse* On-surface reactions are a promising strategy for synthesizing complex architectures that are potentially relevant in the field of novel nanostructures and molecular electronics. Suitable design of molecular building blocks is required in order to assemble functional molecules into stable covalently bound molecular wires. The conductance of individual molecular wires has been investigated as a function of their length by pulling individual wires off the surface by the tip of a scanning tunneling microscope. This reveals detailed insight into the properties and motion of single functional molecules as well as the role of the electronic structure on the charge transport.
14:45	**606**	**STED Lithography Below the Diffraction Barrier** *Richard Wollhofen, Bianca Buchegger, Jaroslaw Jacak, Thomas A. Klar* *Applied Physics, Johannes Kepler University Linz, Altenberger Str. 69, AT-4040 Linz* Two-photon polymerization, optionally combined with stimulated emission depletion (STED) lithography, allows two and three dimensional polymer fabrication with structure sizes and resolution below the diffraction limit. To achieve spatial polymerization restriction similar to STED-microscopy, the excited photoinitiators (fluorophores) are depleted in the outer rim of the excitation volume via stimulated emission by a second laser beam. Thereby, the feature size can be decreased to several tens of nanometers. Currently, feature sizes as small as 55nm and a resolution of 120 nm of adjacent lines can be achieved. Recently, STED lithography allows us to produce well characterized, biocompatible nanoanchors as platforms for single, biochemically active proteins, applicable to many biological assays.
15:00	**607**	**Evaluation of insertion loss of noise barriers with special shapes** *Holger Waubke, Christian Kasess* *Acoustics Research Institute, AAS, Wohllebengasse 12-14, AT-1040 Vienna* Only for straight noise barriers an analytic solution for the insertion loss exists. For noise barriers with arbritary shape and absorptive material a simulation with the boundary element method in 2D gives numerical results. These results are fitted by polynomials depending on the target angle and the source angle to incoporate the results into noise mapping software.
15:15		***END***
15:30		***Coffee Break***

ID	Applied Physics, Geophysics, Atmosphere and Environmental Physics Poster
621	**Direct measurement of axial optical forces** *Martin Bawart, Gregor Thalhammer, Lisa Obmascher, Monika Ritsch-Marte* *Medical University Innsbruck, Division of Biomedical Physics, Müllerstraße 44 , AT-6020 Innsbruck* Measuring forces on the micro-scale with the aid of optically trapped particles provides insight to mechanical properties and processes taking place, e.g., in cells or micro-organisms. We directly measure the optical force based on the change of momentum of the in- and outgoing light, which has the benefits of being independent of particle size, shape, and beam shape. We validated the accuracy of direct force measurements in the axial direction for a single beam optical tweezers setup, based on numerical simulations as well as experimental investigations and found that a good accuracy with an error of less than 1% can be achieved.

622 Covalent bond ruptures in single molecule force spectroscopy

Florian Berger [1], Katharina Holz [2], Michael Pill [3], Ulrich Lüning [2], Martin K. Beyer [1], Alfred Kersch [3], Hauke Clausen-Schaumann [3]
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In this work, bond ruptures of individual molecules are investigated by applying a mechanical force using an Atomic Force Microscope (AFM). In order to specify the point of rupture a cyclic chain is synthesized, involving the covalent bond of interest.[1] After bond rupture, this chain is acting as safety line, increasing the length of the molecule by a known value, which is calculated quantum chemically. Here, two safety lines of different lengths are applied on a cyclobutane mechanophore to validate the method.

[1] Schütze, D.; Holz, K.; Müller, J.; Beyer, M.K.; Lüning, U.; Hartke, B. Angew. Chem. Int. Ed. 2015, 54, 2556-2559.

623 Electroluminescence and photovoltaics in two-dimensional semiconductors

Lukas Dobusch [1], Andreas Pospischil [1], Marco Mercurio Furchi [1], Florian Libisch [2], Joachim Burgdörfer [2], Thomas Müller [1]
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[2] Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstr. 8-10, AT-1040 Vienna

Two-dimensional semiconductors, such as transition metal dichalcogenides offer great opportunities for opto-electronic applications due to their crystalline quality, high stability, and flexibility. We show the implementation of a solar cell, a photodiode and a light-emitting diode based on a tungsten diselenide (WSe_2) monolayer, acting as a p-n junction diode [1]. In another approach, two two-dimensional crystals (molybdenum disulfide (MoS_2) and tungsten diselenide (WSe_2)) were vertically stacked in order to achieve an atomically sharp interface. Under appropriate gate bias, this junction shows a photovoltaic effect upon optical illumination [2].

[1] A. Pospischil, et al.; Nature Nanotech. 9, 257-261 (2014); [2] M. M. Furchi, et al.; Nano Lett. 14, 4785-4791 (2014)

624 Dual-color electronically controlled terahertz time-domain spectroscopy

Vincent Paeder, Juraj Darmo, Karl Unterrainer
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We demonstrate high speed and high resolution terahertz time-domain spectroscopy based on a dual-color electronically controlled optical sampling (ECOPS) system. We combine the extended scanning range available to asynchronous optical sampling and the high resolution of ECOPS with a double-stage electronic control. We highlight the superiority and flexibility of the new technique through various examples.

625 Investigation of tannin-furanic rigid foams by multi-wavelength Raman spectroscopy

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Due to their outstanding physical properties of high fire resistance and low thermal conductivity, tannin-furanic rigid foams are used in multiple innovative applications (e.g. green building technology). These bio-friendly organic materials are polymerized via an acid catalyzed polycondensation reaction between furfuryl alcohol and condensed flavonoids. The aim of this study is to characterize the chemical structure of tannin-furanic rigid foams by multi-wavelength Raman spectroscopy (455 nm, 532 nm, 1064 nm). The obtained spectral signatures are compared with that of the precursor materials and structurally related substances. The thereby observed spectral similarities to several sp2-carbon materials will be discussed.

626 The Enigma Thermochromic Behavior in Tetraalkyle Distibines (R_4Sb_2)

Andreas Reyer [1], Raphael J. F. Berger [1], Daniel Rettenwander [1], Paolo Sereni [1], Maurizio Musso [1], Peter Blaha [2], Thomas Berger [1], Stefan Heimann [3], Stephan Schulz [3]
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[2] Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, AT-1060 Wien
[3] Institute of Inorganic Chemistry, University of Duisburg-Essen, Universitätsstraße 5-7, DE-45117 Essen

Recently, Schulz and coworkers have prepared the tetra ethyl derivative (R = Et) which has two solid modifications showing distinctly differing colors (yellow or red) but both containing chains of [···Et_2Sb-SbEt_2···] molecules with virtually same geometrical structure only differing in modes of chain packing. MO based explanations from Hoffmann and coworkers, where the thermochromic absorption shift was assigned to the formation of intermolecular Sb···Sb contacts in the solid state, are thus not sufficient to describe the thermochromics behavior of distibines. Based on our results from temperature dependent Raman, UV-VIS spectroscopy and DFT calculations we suggest an alternative model, assuming the formation of stibinyl radical defect occupancies in the solid state.

627 Investigation of structural phase transition in the clinopyroxene-type structure of $CaCu_{1-x}Zn_xGe_2O_6$ with Raman spectroscopy

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The investigated clinopyroxene-type structure of $CaCu_{1-x}Zn_xGe_2O_6$ belongs to the class of pyroxenes, with the general formula $M2M1T_2O_6$. Pyroxenes are chain silicates and germanates and the mineral members of this group are very widespread constituents of the Earth Crust and the upper mantle. From X-ray diffraction we know, that $CaCu_{1-x}Zn_xGe_2O_6$ shows a phase transition between $P2_1/c$ and C2/c symmetry by changing Cu content from 0,90 to 0,88 apfu (atoms per formula unit) at 298 K. In this study we follow the structural phase transition in the solid solution series compounds with Raman spectroscopy, both as a function of chemistry and temperature.

628 Photodissociation of ionized Leucine Enkephalin

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In recent years several methods for effective ultraviolet photodissociation of peptides have been implemented. Wilson et al. demonstrated the sequencing of different peptides by attaching a UV-chromophore to the N-terminus. Here a tunable wavelength optical-parametric oscillator (OPO) laser was coupled into a Bruker 9.4T Fourier Transform Ion Cyclotron Mass Spectrometer. Leucine Enkephalin is ionized by electrospray ionization. Photofragments are detected as a function of irradiation wavelength. The influence of the charge carrier, e.g. proton or Na^+ ion, on the photodissociation spectrum is explored.

629 Interaction of sodium iodide clusters with small hydrocarbons

Nina Bersenkowitsch, Martin K. Beyer, Universität Innsbruck, Technikerstraße 25, AT-6020 Innsbruck

Marine aerosols consist of a variety of components and are of great importance for many atmospheric processes, for instance, backscattering of solar radiation via clustered sea salt particles. A Fourier Transform Ion Cyclotron Resonance Mass Spectrometer (FT-ICR MS) is a versatile tool to investigate interactions between clusters and molecules and their photochemistry. With electrospray ionization, sodium iodide clusters with hydrocarbon adducts are produced and interactions with organic compounds are analyzed. For measuring absorption spectra, an optical parametric oscillator is coupled into the 9,4T FT-ICR-MS. Hence, UV/VIS spectra are measured via photodissociation of the given compounds, and the photochemical reaction products are analyzed.

630 Ultrafast dynamics in highly doped plasmonic oxides

Wolfgang Eder, Johannes Ziegler, Meirzhan Dosmailov, Calin Hrelescu, Johannes D. Pedarnig, Thomas A. Klar
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Noble metals as plasmonic materials have a few drawbacks, like high losses or low melting temperature. For photonic devices, e.g. metamaterials, in the near-infrared highly doped transparent conducting oxides such as aluminium doped zinc oxide (AZO) are possible alternatives for noble metals and already proofed to have some advantages compared to conventional metamaterials. We spectrally resolved, from visible to near- infrared, the relative change in transmission ($\Delta T/T$) of highly doped AZO films using femtosecond pump-probe measurements. Our results show an exponential decay on a picosecond time scale.

631 **Modeling of contact erosion for high voltage circuit breakers**

Frank Kassubek [1], Kai Hencken [1], Javier Mantilla [2], Muhammad Jamal Riaz Ahmad [1]
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Erosion of contacts during arcing is an important limiting factor for the lifetime of high voltage circuit breakers. Erosion over many switching events accumulates leading to a change of contact shape that may affect breaker performance. Using empirical models for arc root position and erosion of material, we predict the evolution of the geometric shape of the contacts depending on the current flowing through the device. The results are compared to experimentally measured shapes and reasonable agreement is found for models including heat conductance into the contacts.

632 **Sensitivity of surface interactions in a Single-column Atmosphere-Lake model: a case study**

Stephane Goyette, Marjorie Perroud
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Lakes become essential parameterizations over continental surfaces in numerical models to reproduce regional weather and climate realistically for many regions over the world. However, the local effects of surface-atmosphere processes and their associated feedbacks may not be easily isolated and further analysed. In this study, the role of air–lake interactions in the simulation of the evolution of the surface energy budget is explored using the Single Column atmospheric Model FIZC coupled with a k-e lake model. We investigate numerically the influence of the lake-atmosphere interactions in terms of the factor separation methods in order to explore the effects of nonlinearities upon surface exchanges of energy and mass.

633 **Frequency noise and stabilization of quantum cascade lasers**

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We present a study of the frequency stability of a mid-infrared quantum cascade laser (QCL) as well as preliminary steps towards the frequency stabilization of a QCL onto a micro-resonator for linewidth narrowing. The frequency stability and the evolution of noise in a QCL were continuously measured during a 2-months period and showed a similar behaviour characterized by a drift during the first month attributed to the laser contacts, followed by a stable regime. Mid-infrared chalcogenide fibres were tapered using a home-built setup and are used to couple the QCL into the resonator with QCL-fiber coupling efficiency of 80%.

634 **The Photon Single Shot Spectrometer used at the SwissFEL**

Jens Rehanek, Pavle Juranic, Christian David, Luc Patthey, Paul Scherrer Institut, CH-5232 Villigen PSI

Once the FEL undulator segments are matched, lasing-process starts and the generated radiation needs to be inspected. The resulting spectrum will vary from shot to shot. In order to cover these variations, an X-ray optical apparatus is required, capable to result a spectrum containing the information with a sufficient energy resolution. At the same time the entire system needs to work at very high temporal resolution. The task is, to obtain this information right during performing experiments as an onlinedevice. It should be able to deliver most of the XFEL-generated radiation towards the experiment, getting its spectral information, simultaneously.

635 **Using lensed fibers for stimulating ex-vivo retina: simulation and measurement results**

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We stimulate the ex-vivo mouse retina with an attenuated laser source with a intensity density < 10 photon/(sec. μm^2) via lensed fibers and measure the retina response. There are several challenges for interfacing the tissue with the beam: e.g. the tissue is bathed in buffer solution and the beam size must be well-defined along the retina photoreceptors while the distance between the photoreceptor layer and fiber tip is not exactly fixed. We use ball lensed fibers (with spacer) that fulfill such requirements to a good extent. In this presentation we report the simulation results of such fibers and compare them with the measurement.

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STED Lithography with Functional Clusters

Jaroslaw Jacak [1], Bianca Buchegger [1], Johannes Kreutzer [2], Birgit Plochberger [3], Richard Wollhofen [1], Dmitry Sivun [1], Ulrich Schubert [2], Thomas A. Klar [1]
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STED lithography is a technique used to fabricate acrylic structures with feature sizes far below 100 nm in 3D. However, the difficulty of covalent functionalization remains, since most of these polymerized structures do not possess exposed reactive groups. Selective structure functionalization would be beneficial and would allow a directed coating of the nanoscopic features with for e.g. macromolecules or metals. Herein we show first STED-lithography structures doped with reactive mercapto-groups at different concentrations. Using a 780 nm two-photon excitation laser and a 532 nm CW depletion laser, feature sizes of ~λ/12 have been achieved. The functionality of the mercapto-groups has been proven via specific fluorescent labeling with Alexa647 labeled maleimides.

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Effective Perrin Theory for a Liquid of Infinitely Thin Brownian Needles

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Liquids of infinitely thin Brownian needles of length L are considered up to reduced densities of $n^* = nL^3 = 10^3$ deep in the semidilute regime. To simplify, we consider the dynamics of a single needle in a static environment of other needles and corroborate the scaling behavior n^{*-2} of the diffusion coefficients of a needle liquid. We find excellent agreement between the intermediate-scattering function in the semidilute regime and a full analytic solution for a freely moving rod with the transport coefficients obtained from molecular dynamics simulation as input parameters. We compare the results to a liquid of subsequent moving needles.