O 26: Poster: New Methods

Time: Monday 18:00–20:00 Location: P2/EG

O 26.1 Mon 18:00 P2/EG

Instrumentation for high-resolution biomolecule imaging enabled by electrospray ion beam deposition (ES-IBD) — •Lukas Eriksson, Tim Esser, Márkó Grabarics, Paul Fremdling, and Stephan Rauschenbach — University of Oxford, Department of Chemistry, United Kingdom

Elucidating the structure of biomolecules is essential to understanding their function. Direct imaging with cryogenic electron microscopy (cryo-EM) or scanning probe microscopy (SPM) is a powerful approach for finding molecular structure. However, sample preparation can be a major challenge: either very time- and resource-intensive or incompatible with the vacuum environment required by the imaging method.

Here, we explore preparative mass spectrometry as an alternative workflow towards structural elucidation of biomolecules. A novel, custom-built deposition stage extending a commercial mass spectrometer allows for the mass-filtered, soft-landed deposition of a wide mass range of target molecules (m = 100 - 10^6 amu) onto various surfaces, including cryo-EM grids and metal crystals for SPM.[1] This requires extensive control over conditions such as pressure, temperature, ion trajectories, sample surfaces, and sample transfer to obtain clean, chemically pure samples of the desired species in the right (i.e. native) configuration.

[1] Paul Fremdling, Tim K. Esser, Bodhisattwa Saha, Alexander A. Makarov, Kyle L. Fort, Maria Reinhardt-Szyba, Joseph Gault, and Stephan Rauschenbach: *A Preparative Mass Spectrometer to Deposit Intact Large Native Protein Complexes.* **ACS nano** 16 (2022)

O 26.2 Mon 18:00 P2/EG

Spectral characterization of battery components from Li-ion battery recycling processes — •Julia Richter[1,2], Sandra Lorenz[2], Christian Röder[1], Roman Tschagaew[1], Yuleika Carolina Madriz Diaz[2], Erik Herrmann[2], Richard Gloaguen[2], and Johannes Heitmann[1] — [1]TU Bergakademie Freiberg, Institute of Applied Physics, Leipziger Str. 23, D-09599 Freiberg (Germany) — [2]Helmholtz-Zentrum Dresden-Rossendorf, Helmholtz Institue Freiberg for Resource Technology, Chemnitzer Str. 40, D-09599 Freiberg (Germany)

The rapid identification of critical compounds in recycling material streams is crucial for an adequate sorting. Recently, the development of adapted multi-sensor systems as well as advanced multi-source data fusion for real-time data integration is in the scope of several research activities. This work deals with the digitalisation of mechanical separation processes in recycling of Li-ion batteries using data which were acquired by hyperspectral sensors. In order to establish a reference data set of the valuable components Al and Cu, in this study a sample set of Al and Cu foils was examined by reflectance spectroscopy in the range (350 * 2500) nm. Based on point measurements and statistical data from imaging sensors, optical material characteristics of the samples were analysed. Proposals for optical sorting steps and possible challenges will be outlined and discussed. This work is financially supported by the Federal Ministry of Education and Research (BMBF) in the framework of the greenBatt cluster within the project DIGISORT.[1] [1] www.greenbatt-cluster.de/de/projekte/digisort/

O 26.3 Mon 18:00 P2/EG

Dynamics of contact electrification — •Andre Mölleken, Hermann Nienhaus, and Rolf Möller — Fakultät für Physik, Universität Duisburg-Essen, Germany

Although the electrical charging of objects brought into contact has been observed for centuries, the details of the underlying mechanism are still not yet fully understood. We have developed an experimental method to follow the charge of a small sphere bouncing on a grounded planar electrode on a time scale down to 1 μs. In case of a contact between two metals, it reveals that the sphere is discharged in the moment of contact, which lasts about 6 to 8 μs. However, at the very moment of disruption of the electrical contact, it regains charge far beyond the expectation according to the contact potential difference. The excess charge rises with increasing contact area.

[1] M. Kaponig, A. Mölleken, H. Nienhaus, R. Möller, Dynamics of contact electrification, Sci. Adv. 2021, 7 (22), eabg7595.

O 26.4 Mon 18:00 P2/EG

Surface tension measurement of pure water in vacuum — •Paul T. P. Ryan, Jiri Pavelec, Jan Balajka, Michael Schmid, and Ulrike Diebold — Institute of Applied Physics, TU Wien, Austria

Very little is known about the surface tension of pure liquids in contact with their pure gaseous phases, i.e. without the presence of other gases or liquid phase contaminants. This is surprising given that contaminants are known to greatly affect surface tensions values[1]. Recently we have developed a method to dose liquid water onto pristine surfaces in UHV using a small cryostat[2]. We combine this approach with the pedant drop method[3] to measure the surface tension of ultra-clean liquids in contact with their pure gaseous phases. In the design, the ultra-clean liquid is condensed onto a small cryostat placed in a vacuum chamber. A pendant drop is formed and carefully photographed allowing the surface tension of the ultra-clean liquid to be directly determined. For these types of measurements accurate knowledge and control of the temperature, pressure and the optics of system is of paramount importance. How these parameters are precisely controlled in the instrument design will be discussed along with initial measurements of ultra-pure water. [1] Yuki Uematsu, et. al., Current Opinion in Electrochemistry, Volume 13, (2019) [2] Jan Balajka, et. al., Science, 361, (2018) [3] Berry, J. D. et. al., J. Coll. Interface Sci. 454, (2015).

O 26.5 Mon 18:00 P2/EG

High-Resolution Imaging of Protein Complexes Enabled by Electrospray Ion-Beam Deposition Sample Preparation — •Asha Thompson, Tim Esser, Markó Grabarics, Isabelle Legge, and Stephan Rauschenbach — University of Oxford, Department of Chemistry, United Kingdom

Structural characterisation of biological molecules such as proteins is essential for insight into their processes and interactions within cells. Samples of mass-filtered molecules adsorbed onto surfaces can be obtained using preparative mass spectrometry techniques such as electrospray ion-beam deposition (ES-IBD). ES-IBD generates intense beams of native proteins which are soft-landed onto surfaces. This produces uncontaminated samples which can be further characterised by transmission electron microscopy (EM) or scanning probe microscopy (SPM).

Here we present the application of this approach for the imaging of proteins showing examples of soluble and of membrane proteins, such as Human C Reactive protein, ferritin, Beta-galactosidase and Aquaporin-Z. We can show that the shape of the protein, its subunit conformation, and stoichiometry are retained, which points to intact secondary structure. [1] We intend to extend this approach to map the interactions of antibodies and their targets in order to provide information about the binding sight, useful for pharmacology.

[1] T. K. Esser, et al, Mass selective and ion-free electron cryomicroscopy protein sample preparation, PNAS nexus, Volume 1, issue 4, 2022

O 26.6 Mon 18:00 P2/EG

RuNNer 2.0: An efficient and modular program for training and evaluating high-dimensional neural network potentials — •Alexander L. M. Knoll[1,2], Marco Eckhoff[3], Jonas A. Finkler[4], Tsz Wai Ko[5], Emir Kocer[1,2], K. Nikolas Lausch[1,2], Moritz R. Schäfer[1,2], Gunnar Schmitz[1,2], Alea Miako Tokita[1,2], and Jörg Behler[1,2] — [1]Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany — [3]ETH Zürich, Laboratorium für Physikalische Chemie, 8093 Zürich, Switzerland — [4]Department of Physics, Universität Basel, 4056 Basel, Switzerland — [5]Department of NanoEngineering, University of California, San Diego, CA, USA

Machine learning potentials (MLPs) have become a popular tool for large-scale atomistic simulations in chemistry and materials science. They provide efficient access to highly accurate potential energy surfaces (PES) generated from *ab initio* reference calculations. As methods in this field are becoming increasingly complex and reach maturity, the development of efficient and user-friendly tools is also gaining importance. We present the second major release version of RuNNer, an open source, stand alone software package for the construction and evaluation of second, third, and fourth generation high-dimensional neural network potentials (HDNNPs). RuNNer 2.0 unifies an entire workflow in a fully MPI-parallel program: from the generation of atomistic descriptors, over the training of a specific machine learning model, to its final application in molecular dynamics codes.

O 26.7 Mon 18:00 P2/EG

Optical Near-field Electron Microscopy — •Ilia Zykov[1], Hanieh Jafarian[1], Barbara Platzer[1], Thomas Juffmann[1], Amin Moradi[2], Guido Stam[2], Sense Jan van der Molen[2], Ruud Tromp[2], Nestor Fabian Lopez Mora[3], Mariana Manuela Amaro[3], Martin Kalbac[3], Martin Hof[3], and Radek Šachl[3] — [1]University of Vienna, Austria — [2]Leiden University, the Netherlands — [3]J. Heyrovsky Institute of Physical Chemistry, the Czech Republic

Lable- and damage-free imaging of the surface processes on the nanometer scales and over extended periods is required in different fields. Various electron microscopy techniques are applied to meet these requirements. However, the use of electrons in probing the sample may affect some specimens. The novel Optical Near-field Electron Microscopy (ONEM) technique [1] is being developed to overcome this drawback. In the ONEM light nondestructively interacts with a sample. The scattered light from the sample is then transformed into electrons by a nm-thick photocathode layer placed in the near-field region of the sample. The nm resolution images are then achieved through an electron readout using the Low Energy Electron Microscope.

The potential application of ONEM in biochemistry can be to follow the protein dynamics in lipid membranes at single protein resolution. In electrochemistry ONEM will be applied to study the nucleation and growth of nanoscale copper clusters without any electron beam effect.

[1] R. Marchand et al, Phys. Rev. Applied 16, 014008 (2021)

O 26.8 Mon 18:00 P2/EG

Development of a reflektometer for polarised surface sensitive X-ray Absorption Spectroskopy — •Lukas Voss, Frederic Braun, Franz Eckelt und Dirk Lützenkirchen-Hecht — Bergische Universität Wuppertal, Wuppertal, Deautschland

ReflEXAFS measurements represent a powerful tool for surface-sensitive structure investigations. With the help of high-intensity synchrotron radiation on synchrotron beamlines of the third generation, this measurement method can also be used in a time-resolved mode. In order to keep the construction and adjustment time as short as possible, a simple, compact and transportable reflectometer is to be built in order to give other users easy access to this measurement technology. Here we would like to present the current status of the project with the first measurements.