O 66: Poster: Nanostructures at Surfaces

Time: Wednesday 18:00–20:00 Location: Poster C

O 66.1 Wed 18:00 Poster C

Direct electron beam patterning of electro-optically active PEDOT:PSS for switchable metasurfaces — •Dominik Ludescher[1], Siddharth Doshi[2,3], Julian Karst[1], Moritz Floess[1], Johan Carlström[3], Bohan Li[3], Nofar Mintz Hemed[2], Yi-Shiou Duh[3], Nicholas A. Melosh[2], Mario Hentschel[1], Mark Brongersma[3] und Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, United States — [3]Geballe Laboratory for Advanced Materials, Stanford University, 476 Lomita Mall, Stanford, CA 94305, USA

Conducting polymers, exemplified by PEDOT:PSS, exhibit distinctive electronic and polymeric attributes. When subjected to CMOS-compatible voltages, PEDOT:PSS transitions between insulating and metallic states via an intrinsic electrochemical redox reaction. Consequently, these materials are suited perfectly for AR/VR applications, advanced display technologies, and dynamic sensors. Harnessing the full potential, however, demands a robust foundation in fabrication techniques. Historically, electron-beam lithography was utilized to generate a resistant etch mask, albeit with fabrication complexities. To circumvent some of these challenges, we present a novel and alternative fabrication method. This concept is based on the electron-beam induced water solubility modulation due to crosslinking between the PEDOT:PSS polymer chains. With this approach nano-wire structures with a width of down to 250 nm can be achieved.

O 66.2 Wed 18:00 Poster C

Enhancing Chiroptical Sensitivity: Exploring Chirality with Second Harmonic Generation-Circular Dichroism Spectroscopy — •Charitini Panagiotopoulou, Kevin Liang, Changseop Jeong, Ueli Heiz, and Aras Kartouzian — Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany

Chirality holds significance in a variety of molecules, playing a fundamental role in chemical, biological, and material processes. Circular Dichroism (CD) spectroscopy, utilizing circularly polarized light, discloses the differential in absorption between right and left circularly polarized light. Chiral molecules, featuring non-superimposable mirror images, necessitate CD for rapid, non-destructive analysis of their structural and electronic properties. Our study introduces a method to enhance CD sensitivity; Second Harmonic Generation (SHG) spectroscopy, known as SHG-CD spectroscopy. This approach uses the nonlinear response of SHG, which is particularly effective in non-centrosymmetric environments like thin film surfaces. Under UHV conditions, we investigate the structural aspects of chiral molecules on thin films and the chirality transfer to achiral counterparts, making a wide range of applications possible, from fundamental studies of surface properties to practical applications in fields such as materials science, biophysics, and catalysis.

O 66.3 Wed 18:00 Poster C

Measuring the local surface potential of ionic liquids layers upon charge deposition — •Mirco Wendt[1,2], Regina Lange[2], Jens Berdermann[1], Ingo Barke[2], and Sylvia Speller[2] — [1]Institute for Solar-Terrestrial Physics, German Aerospace Center (DLR), Kalkhorstweg 53, 17235 Neustrelitz — [2]Institute of Physics, University of Rostock, Albert-Einstein-Str. 25 18059 Rostock

The interaction of ionic liquids (IL) with surfaces at different potentials is extensively studied with respect to their potential application in double layer capacitors[1,2]. The surface potential of the liquid itself, however, is rarely investigated[3], although it was shown that electrostatic screening in IL does not adhere to well established models for low concentration electrolytes[4]. We show how the local surface potential of 1-Butyl-1-methyl-pyrrolidinium- dicyanamide (BMP DCA) can be measured in ultra-high vacuum, using a q-Plus-Sensor in a Kelvin-Probe-like configuration. We address implications and assets of this approach and discuss its application to BMP DCA thin films on floating gold islands on top of glass. To modify the native surface potential, patches of this film were exposed to the electron beam of a scanning electron microscope and show both temporary and permanent contrast differences upon prolonged exposure. Studying the local surface potential of such patches and its evolution should allow for a better understanding of mechanisms involved.

[1] Thangavel, et al., J. Power Sources 2018 [2] Han, et al., Adv. Mater. Interfaces 2020 [3] Zhang, et al., Acta Phys. Chim. Sin. 2016 [4] Gebbie, et al., Proc. Natl. Acad. Sci. 2013

O 66.4 Wed 18:00 Poster C

Plasma Treatment of Electrode Surfaces — •Joshua Nicolai Maruschtschyn[1], Timo Wagner[1], Nicolas Wöhrl[1], Vineetha Vinayakumar[2], Christian Marcks[3], Anna Mechler[3], Doris Segets[2], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Particle Science and Technology (IVG-PST) and CENIDE, University of Duisburg-Essen — [3]AVT.ERT, RWTH Aachen University

In the planned transition toward a CO2 neutral economy and industry, hydrogen plays a significant part. In the production of hydrogen catalysis is of great importance, necessitating better and cheaper catalysts. To make high-performance electrodes cheaper, they will need to be produced in series. To establish this the H2Giga project was started. One promising method here in is the plasma treatment of the electrodes, with which various material properties can be enhanced, such as increasing the surface area or improving the adhesion of catalyst particle coatings. The method is viable for scaling and roll to roll production. The experimental setup and procedure used for the plasma treatment is discussed. Various electrode materials are treated, such as nickel, nickel with catalyst particle coatings, copper and others. The results are investigated using a scanning electron microscope, electrochemical tests and adhesion tests. The results are presented and possible future steps are discussed.

O 66.5 Wed 18:00 Poster C

Direct two-photon laser structuring of electrically switchable PEDOT:PSS for nanophotonics — •Pavel Ruchka, Dominik Ludescher, Leander Siegle, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

Switchable conducting polymers, such as PEDOT:PSS, have recently seen a growing interest, as they promise new possibilities for compact integrated devices in augmented/virtual reality applications, nanophotonics, and other fields of optics. Typically, such materials are structured by imposing and etching resist-masks, which can be tedious, costly, and time-consuming. Here, we present a new method to fabricate switchable micro- and nano-structures from PEDOT:PSS using direct laser writing by two-photon lithography. We study the resolution that can be achieved with this technique and demonstrate electrical switching of the optical properties of the obtained structures. As an example, a simple grating with sub-micrometer linewidth is produced and switched, resulting in an electrically switchable nanophotonic beam-steering device, which can be benchmarked to already existing fabrication methods.

O 66.6 Wed 18:00 Poster C

Design of femtosecond nanostructured stainless steel orthopedic implants, magnetron sputtered with Cu and optimized for calcium phosphates crystals growth for application in orthopedics — •Liliya Angelova[1], Albena Daskalova[1], Maja Sikiric[2], and Tihomir Car[2] — [1]Institute of Electronics, Bulgarian Academy of Sciences, 1784 Sofia, Bulgaria — [2]Ruder Bošković Institute, 10 000 Zagreb, Croatia

Nowadays, the engineering of load-bearing bone tissue after severe trauma still relies on metal-based permanent implants. Such artificial tissues are usually applied in the body and come into direct contact with the recipient's cells, whose adhesion directly affects the acceptance or rejection of the implant by the patient. The present study aims to create nano rough texture employing ultra-short femtosecond laser (fs)-induced periodicity in the form of LIPSS on the surface of a mechanically stable stainless steel implant model, that is additionally functionalized by magnetron sputtered Cu thin layer, giving the as created implants stable antimicrobial surface interface. Calcium phosphate (CaP) crystal growth was additionally performed due to the well-known high mechanical stability and load-bearing properties

that CaPs give to the bone connective tissue, as well as for the strong interface bond that they make between the artificial implant and the surrounding bone tissue, stabilizing in that way the implanted structure in the body. The optimization of the bioactive properties of the as-created antimicrobial hybrid topographical design has the potential for subsequent practical application in bone tissue engineering.

O 66.7 Wed 18:00 Poster C

Dewetting of Thin Gold Films on Flat and Nanostructured Polystyrene Surfaces — •Felix Lohmeyer, Daniel Kool, Philipp Hodges, and Jörg K. N. Lindner — Nanopatterning - Nanoanalysis - Photonic Materials, Department of Physics, Paderborn University, Germany

Limited knowledge exists regarding the wetting and dewetting behavior of ultra-thin metal films on polymer surfaces, although this understanding is crucial for advancing nanotechnology processes. We show that dewetting of thin metal films occurs below the polymer's melting point making it valuable for patterning purposes. We present preliminary results for 7 nm thin gold films deposited on polystyrene after thermal annealing. Different polymer substrates, including planar polystyrene films, a phase-separated PS-b-PMMA block-copolymer with a fingerprint nanostructure, and a nanostructured polystyrene surface obtained by selectively removing the PMMA matrix from an ordered block-copolymer film, are explored.

Dewetting degree is examined as a function of annealing time and temperature. The fraction of Au-covered surface is larger on fingerprint-patterned PS-b-PMMA surfaces than on pure planar PS films. On nanostructured PS films, gold decomposes upon annealing into rods, both on top of the PS fins and in the pattern valleys. These results illuminate the potential of dewetting on polymers for nanotechnology purposes.

O 66.8 Wed 18:00 Poster C

Photoinduced dynamics of plasmonic HfN nanodots and thin films — •Marc Herzog[1], Maximilian Mattern[1], Alexander von Reppert[1], Steffen Zeuschner[1], Matthias Rössle[1], Florin Boariu[1], Jan-Etienne Pudell[2], Angel Rodriguez-Fernandez[2], Wonhyuk Jo[2], Anders Madsen[2], Sven Askes[3], Andrea Baldi[3], and Matias Bargheer[1,4] — [1]Institut für Physik, Universität Potsdam, Germany — [2]European XFEL, Germany — [3]Vrije Universiteit Amsterdam, Netherlands — [4]HZB Berlin, Germany

Metallic nanoparticles can be exploited to focus light energy onto the nm scale where it may trigger specific processes such as chemical reactions. The "gold standard" in nanoplasmonics, i.e. Au nanoparticles, suffers from the superior electron heat conductivity which quickly spreads the absorbed nanofocused energy away from the hot spots. Hafnium nitride (HfN) is a very robust material and its plasmonic properties and large electron-phonon coupling facilitate a light-generated long-lived nanofocusing of heat rendering it a very promising material in plasmon-assisted catalysis.

The knowledge of the local temperature in nanoparticles is critical for a thorough understanding of light-driven nanoscale processes, however, its experimental determination is by no means straightforward. Using ultrafast x-ray diffraction, we compare the photoinduced coherent and incoherent expansion dynamics of HfN thin films and substrate-supported nanodots. We thereby shed light on the morphology dependence of nanooptical and thermoelastic properties of HfN nanostructures.

O 66.9 Wed 18:00 Poster C

An intermediate morphology in the patterning of the crystalline Ge(001) surface induced by ion irradiation — •Denise J. Erb[1], Daniel A. Pearson[2], Tomas Skeren[3], Martin Engler[1], R. Mark Bradley[4], and Stefan Facsko[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Pennsylvania State University, USA — [3]Czech Technical University in Prague, Czech Republic — [4]Colorado State University, USA

We investigate the self-organized nanopattern formation of the Ge(001) surface induced by ion beam bombardment at elevated surface temperatures. Two previously-observed kinds of topographies are seen, i.e., anisotropic patterns of rectangular pyramids and isotropic patterns of shallow round basins [1]. In addition, we unexpectedly observe an intermediate type of pattern, in which isolated rectangular pyramids stand above a landscape of shallow basins. The observed morphology depends on the chosen ion energy and flux and surface temperature. To model the observed pattern morphologies, we extend the equation of motion to include a second order correction term resulting from the curvature dependence of the sputter yield from a patterned surface [2]. This term produces the isolated peaks in the intermediate patterns, while the formation of spike singularities is averted by the Ehrlich-Schwoebel effect. For a range of parameter values, the resulting continuum model of the surface dynamics produces patterns that are remarkably similar to the experimentally observed morphologies (manuscript in review). [1] X. Ou et al., Phys. Rev. Lett. 111 (2013) [2] R.M. Bradley and G. Hobler, J. Appl. Phys. 129 (2021)

O 66.10 Wed 18:00 Poster C

Argon ion induced nanostructuring on Titanium surfaces — •Jens Bauer, Hannaneh Hosseini, Gregor Dornberg, Frank Frost, and Andriy Lotnyk — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

A flexible processing tool to fabricate different kinds of nanostructured surfaces in form of ordered fields of nano-dot or nano-ripple structures is ion-beam erosion by low-energetic ions. A broadband argon ion beam at 1.5 keV is used to investigate the nanostructure formation on polished, polycrystalline cp-Ti samples. The morphology is analyzed by white light interferometry (WLI), atomic force microscopy (AFM), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Electron back-scatter diffraction (EBSD) experiments are performed to analyze the local crystal structure. Under normal ion incidence conditions the ripple morphology is found to be correlated to the crystallographic orientation of the titanium grain structure. Ordered nano-ripples with saw-tooth cross-section are formed with a structure period of 20 – 350 nm and a height of 4 – 50 nm. At low structure periods < 25 nm the ripple morphology tends to unclench resulting in chains of ordered nano-dot arrays. The structure evolution is investigated in the fluence range of 0.3 – 2.0 x 10^{19} $1/cm^2$. The ripple formation on Ti is observed to be time independent indicating a convergent structuring process at normal ion incidence.

O 66.11 Wed 18:00 Poster C

Defect formation in 2D materials by irradiation with highly charged ions — •Lucia Skopinski, Yossarian Liebsch, Stephan Sleziona, Leon Daniel, Lars Breuer, and Marika Schleberger — Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Duisburg, Germany

Two-dimensional (2D) materials, in particular transition metal dichalcogenides, are known for their unique properties. Under bombardment with highly charged ions (HCIs), these materials are modified by targeted defects, allowing tuning of desired properties. Our study addresses the fundamental mechanisms governing the interaction between HCIs and 2D-MoS_2 on different substrates. Each HCI possesses both kinetic and potential energy due to its velocity and charge state, leading to changes such as sputtering of particles upon impact with the material surface. However, a full understanding of the underlying mechanisms is still under discussion.

An in-depth analysis of the emission of secondary ions and atoms aims to unravel the importance of potential and kinetic energy for the underlying nuanced processes. The measured distributions allow a distinction between sputtering driven by the potential and the kinetic energy of the primary ion. The low velocities of the emitted particles suggest an interaction mechanism related to electron-phonon coupling. Furthermore, a comparative study of STEM measurements for pores in 2D-MoS_2 irradiated on a substrate and free-standing provides insight into the influence of the substrate on the modification of the 2D material.

O 66.12 Wed 18:00 Poster C

Microscopic and Magnetic Analysis of Iron Oxide Core-Shell Nanoparticles with Variable Core/Shell Ratio — •Aladin Ullrich, Michael Kühn, and Manfred Albrecht — Universität Augsburg, Universitätsstr. 1, 86159 Augsburg

Cubic iron oxide nanoparticles of about 15 nm were prepared by thermal decomposition of an iron oleate precursor in 1-Octadecene [1]. From scanning transmission electron microscopy and electron energy loss spectroscopy (EELS) measurements a core-shell composition of the particles was found. The particles show a wustite like structure in the core and a spinel like structure in the shell that is indicated from signatures in the EELS spectra [2]. Both, the position of the Fe $L_{2,3}$ white lines and the oxygen fingerprint structure were investigated. By successive oxidation of the particles under a controlled atmosphere, the core/shell ratio could be adjusted up to the complete disappearance of the core. The magnetic properties of this antiferromagnetic core - ferrimagnetic shell system were investigated for a sample series with

core/shell ratios from about 0.3 to zero. The change of the magnetic properties like the blocking temperature, the coercivity, and the exchange bias field was investigated. Magnetic memory measurements following different protocols show clear memory effects and, hence, indicate the presence of a super spin glass state in the samples.

[1] A. Ullrich, M. M. Rahman, A. Azhar, M. Kühn, M. Albrecht, Nanoprticle Research **24**, 183 (2022). [2] A. Ullrich, M. M. Rahman, P. Longo, S. Horn, Scientific Reports **9**, 19264 (2019).

O 66.13 Wed 18:00 Poster C

Plasmonic nanoparticles on silicon: photoemission characteristics and control — •Waqas Pervez, Kevin Oldenburg, Sylvia Speller, and Ingo Barke — Institute of Physics, University of Rostock

Laser excitation of localized plasmons in nanoparticles can give rise to a vastly enhanced photoemission yield [1, 2]. Here we study detailed characteristics of the photoelectron emission process of size-selected nanoparticles with diameters around 10 nm, deposited from the gas phase on silicon. To this end we employ femtosecond laser excitation in a photoemission electron microscope (PEEM). The emission intensity is investigated as a function of space, emission angles, laser wavelength and polarization. We discuss how these parameters can be used to control the electron emission from individual particles. Furthermore, we propose experiments based on a two-color setup which should enable various excitation schemes and reveal phase effects leading to anisotropic electron emission, in analogy to the case of free particles [3].

[1] M. Rohmer et al., Phys. Stat. Solidi B 247, 1132 (2010)
[2] K. Oldenburg et al., J. Phys. Chem. C 123, 1379 (2019)
[3] J. Passig et al., Nat. Commun. 8, 1181 (2017)

O 66.14 Wed 18:00 Poster C

Al-based anodes with high reversible capacity for Li-ion battery — •Kangzhe Cao[1,2], Huiqiao Liu[2], Jiahui Ma[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]College of Chemistry and Chemical Engineering, Xinyang Normal University, Xinyang 464000, China

Aluminum (Al) can alloy with Li at a lithiation potential of ~0.2 V to form LiAl, offering a theoretical capacity of 993 mAh g-1. Moreover, the merits of high electronic conductivity, abundant resources, and environmental benignity endow the Al anode competitive for Li-ion batteries (LIBs). However, the natural Al2O3 passivation layer leads to a large voltage dip (0.1 V), which would interrupt the lithiation process and result in a limited capacity. Meanwhile, the volume expansion (97 %) always makes the electrode in an unstable structure. Herein, we demonstrate a neat avenue to replace the inactive Al2O3 layer with active Sn at room temperature and further encapsulate them into the carbon-based matrix for LIBs. Not any acid or tedious process is needed. Benefiting from the elimination of Al2O3 and the cooperation of carbon matrix, the as-prepared Al-based anodes (Al@Sn@GO pellets and Al@C-Sn pellets) exhibit little voltage dip (0.03 V), higher reversible capacities, and longer cycling life compared to the commercial Al pellet electrode. Considering the low-cost, energy-saving, and facile scalable preparation of the Al-based anodes, our work presents an attractive vision for the development of the practical Al-based anode.

O 66.15 Wed 18:00 Poster C

Optimization of incommensurate organic/inorganic interface structures to study superlubricity — •Lukas Hörmann[1], Johannes J. Cartus[2], and Oliver T. Hofmann[2] — [1]University of Warwick, Coventry, UK — [2]Graz University of Technology, Graz, Austria

Friction is a significant source of energy loss in mechanical devices. One way to reduce this loss is by achieving superlubricity * extremely low friction. Conventional wisdom suggests that incommensurate interface structures facilitate superlubricity. Accurately describing friction necessitates precise first-principles modelling of the interface structure, which is particularly challenging for organic/metal interfaces due to their tunability and propensity for incommensurate structures. However, simulations of incommensurate structures require large system sizes making such calculations intractable. We address this challenge by developing a machine-learned interatomic potential capable of accurately determining energies and forces for structures containing thousands to tens of thousands of atoms. With this approach, we quantify the breakdown of low-friction states in incommensurate structures caused by static distortion waves. Furthermore, we extract design principles to engineer incommensurate interface systems that suppress the formation of static distortion waves, enabling lower friction coefficients.

O 66.16 Wed 18:00 Poster C

Modification of Single-Walled Carbon Nanotubes Using MeV Heavy Ions — •Ayman Sherif El-Said[1], Rene Heller[2], and Stefan Facsko[2] — [1]Physics Department and Interdisciplinary Research Center for Advanced Materials, KFUPM, Dhahran 31261, Saudi Arabia — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01328 Dresden, Germany

Highly energetic heavy ions are used efficiently for tailoring the properties of various nanomaterials [1]. Among the recently investigated advanced materials, the carbon-based ones have attracted a lot of interests due to their promising properties for a wide variety of technological applications [2]. Here, we focus on the structural modifications of single-walled carbon nanotubes (SWCNTs) by irradiation with MeV iodine ions from the tandem accelerators at the Ion Beam Center of HZDR. The ion irradiation leads to fragmentation of the nanotubes into broken segments after surpassing of a specific ion-fluence threshold [3]. Moreover, the Raman spectroscopic measurements show that the disorder parameter increases as a function of ion fluence. Different approaches are discussed for the explanation of the mechanisms responsible for the observed ion-induced changes in SWCNTs.

[1] F. Aumayr, S. Facsko, A.S. El-Said, C. Trautmann, M. Schleberger, J. Phys.: Condens. Matter 23, 393001 (2011).
[2] F.L. Michael et al., Science 339, 535 (2013).
[3] A.S. El-Said, S. Rao, S. Akhmadaliev, S. Facsko, Phys. Rev. Applied 13, 044073 (2020).

O 66.17 Wed 18:00 Poster C

Surface engineering via an ultrathin alumina membrane for constructing stable sodium metal anodes — •Jiajia Qiu, Changfan Xu, Yu Duan, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Despite the high theoretical specific capacities (1166 mAh g-1) and low redox potentials (-2.71 V vs. normal hydrogen electrode) of Na metals, unstable solid electrolyte interphase (SEI) remains a major bottleneck due to the mossy or dendritic growth of Na in the repetitive stripping and plating process of sodium metal batteries. Owing to chemical and electrochemical stability during electrochemical plating and stripping, the Al2O3 coatings enable reduced Na dendrite growth. Simultaneously, the ultrathin alumina membrane (UTAM) network can change the traditional nucleation and growth modes from the origin, which can provide a porous 3D host to accommodate the large volume change of the Na anode. As a result, the UTAM network significantly improved Coulombic efficiency while avoiding short-circuit risks. This novel design may bring in new opportunities for next-generation high-performance Na metal batteries.

O 66.18 Wed 18:00 Poster C

Confinement and band dispersion of excited surface electrons in a two-dimensional porous network on a metallic surface — •Lukas Kau, Martin Mitkov, Ralf Hemm, Lyu Lu, Martin Anstett, Martin Aeschlimann, and Benjamin Stadtmüller — University of Kaiserslautern-Landau and Research Center OPTIMAS, Erwin-Schrödinger Str. 46, 67663 Kaiserslautern, Germany

Two-dimensional metal-organic networks (MONs) on noble-metal surfaces are highly tuneable porous architectures for designing the electronic properties of surfaces by quantum confinement. In this study, we investigate the electron confinement and the corresponding band structure of the excited surface electrons, i.e. the image potential state (IPS), in a self-assembled Cu-coordinated T4PT porous network on a Cu(111) surface. Using two-photon photoemission spectroscopy, we are able to map the band dispersion of the IPS, which reveals a remarkably flat band dispersion and a large effective band mass of approximately $2m_0$. Compared to the occupied Shockley electrons, the excited electrons in the IPS exhibit a strong confinement in the Cu-T4PT porous network [1]. This substantially different confinement of the Shockley surface and the IPS electrons is rooted in the vertical potential landscape of the network structure. Finally, we provide a first glimpse into the hot electron dynamics of the IPS.

[1] Lyu, Lu, et al. arXiv preprint arXiv:2307.06814 (2023)

O 66.19 Wed 18:00 Poster C

Structural Characterisation via X-ray Standing Wave Anal-

ysis: Reactions of Tetraphenyl Porphyrin — •Eleanor S. Frampton[1], Chris J. Judd[2], Matthew Edmondson[2], David A. Duncan[3], Robert G. Jones[2], and Alex Saywell[2] — [1]MAX IV Laboratory, Lund, Sweden — [2]School of Physics, University of Nottingham, UK — [3]Diamond Light Source, UK

Surface-confined reactions offer alternative synthetic pathways to solution-based chemistry and can be studied with a range of techniques to gain deep insights into the on-surface processes taking place during the chemical reaction. By employing a variety of analysis methods a route to understanding and characterizing the mechanistic details of these processes becomes available. This insight provides the tools required to potentially control the selectivity and efficiency of these reactions as well as to design systems with specific functionality.

Here I will focus on how the NIXSW technique can be utilized in combination with STM and XPS. The example system of tetraphenyl porphyrin (TPP) on Au(111) is used to describe how the combination of these methods can lead to a detailed model of an on-surface system, including adsorption geometries of individual molecules. This system consists of three distinct phases, resulting from consecutive on-surface reactions. The chemical specificity of XPS and NIXSW afford us insight into the chemical and structural changes exhibited by the nitrogen atoms within the TPP molecule at each reaction stage. [1,2]

[1] Woodruff, D. P. (2005), Rep. Prog. Phys., 68(4), 743 [2] Frampton, E. S....& Saywell, A. (2023), Inorg. Chim. Act., 558, 121718

O 66.20 Wed 18:00 Poster C

Imaging charge carriers generation process in 2D semiconducting perovskite material — •Dmitrii Sychev[1,4], Andrei Mitrofanov[1,2], Khrystyna Rymsha[1], Karina Zakirova[1], Petr Formanek[1], Darius Pohl[3], Eva Bittrich[1], Quinn Besford[1], Brigitte Voit[1,2], and Ilka Hermes[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden, Germany — [2]Chair of Organic Chemistry of Polymers, Technische Universität Dresden, 01069 Dresden, Germany — [3]3Dresden Center for Nanoanalysis (DCN), Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01069 Dresden, Germany — [4]Technische Universität Dresden, Helmholtztraße 10, Dresden 01062

Organic-inorganic halide perovskites have found their application as photodetectors. The transition from bulk to 2D material enables a greater variety of possible compositions as well as their functionalities.

Here, we investigated novel thin (nanometer scale) particles of halide perovskite semiconducting 2D material for their potential application as photodetectors. Kelvin probe force microscopy (KPFM) is well suited for this purpose, revealing local contact potential. KPFM measurements were performed under 405 and 458 nm illumination. The measurements show a significant decrease in the surface potential of the particles under light. This photoresponse demonstrates the suitability of the material for photodetection applications.

O 66.21 Wed 18:00 Poster C

Collective Radial Breathing Modes in Homogeneous Nanotube Bundles — •Charlotte Berrezueta-Palacios[1], Dekel Nakar[2], Anna Wroblewska[3], Oisín Garrity[1], Han Li[4,5], Nitzan Shadmi[2], Benjamin S. Flavel[4], Ernesto Joselevich[2], Stephanie Reich[1], and Georgy Gordeev[1,6] — [1]Department of Physics, Freie Universität Berlin, Germany. — [2]Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel — [3]Faculty of Physics, Warsaw University of Technology, Poland — [4]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany. — [5]Department of Mechanical and Materials Engineering, University of Turku, Finland — [6]Department of Physics and Materials Science, University of Luxembourg, Luxembourg.

We present a Raman study of the collective vibrations arising from the homogeneous bundling of single-walled carbon nanotubes and analyze the dependence of their vibrational coupling on the tube diameter using two systems, single-walled carbon nanotube coils and a monochiral CNT film. We report on two breathing-like modes for quasi-infinite bundles, compared to the single radial breathing mode characteristic of isolated tubes. The exciton-phonon coupling in these modes is probed with resonant Raman spectroscopy, revealing the same resonance energy for both breathing-like peaks. Our experimental findings align well with previously reported theoretical studies, demonstrating a $1/d$ scaling for all modes, as well as confirming the relative shift of the modes dependent on intertube interaction.

O 66.22 Wed 18:00 Poster C

MBD+C: how to include metallic character (Type C non-additivity) into atom-based dispersion energy schemes — •Alberto Ambrosetti[1] and John Dobson[2] — [1]Università degli Studi di Padova (Italy) — [2]Griffith University (Australia)

Dispersion (van der Waals, vdW) interactions in low-dimensional metals are known to exhibit anomalous "Type -C non-additivity" [Int. J. Quantum Chem. 114, 1157 (2014)] resulting in behavior that is missed by popular atom-based schemes for dispersion energy calculations. For example, the vdW interaction energy between parallel metallic nanotubes at separation D falls off as approximately D^{-2}, whereas current atom-based schemes predict D^{-5}. Here we show how to include Type C effects efficiently within atom-based schemes such as "Many Body Dispersion" (MBD) and "universal MBD" (uMBD). We apply our technique to calculate the van der Waals interaction between parallel metallic chains of gold atoms.