O 71: Poster: Plasmonics and Nanooptics

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

O 71.1 Wed 18:00 Poster D

Light-driven Microdrones — •Carsten Büchner, Jin Qin, and Bert Hecht — Nano-Optics & Biophotonics Group, Experimental Physics 5, University of Würzburg, Germany

The precise manoeuvring of microscopically small objects is a major component of today's microrobotics research and promises a wide range of applications in areas such as micromanufacturing or medicine. Most microrobots use magnetic, acoustic or chemical methods to generate the required propulsion. Here, we demonstrate the fabrication and steering of microdrones that are controlled solely by optical forces in unfocussed light fields. The architecture of the microdrones with a lateral size of approximately 2 um and a mass of 2 pg is comparable to recreational drones and can be realised with two or four motors. The nanomotors, which are individually addressable chiral plasmonic nanoantennas, resonantly scatter the circular polarization components of the driving light into well-defined directions, thus achieving thrust exclusively by photon recoil forces. Two overlapping unfocused light fields of 830 and 980 nm wavelength are used to address the motors. This allows the microdrone to operate in 2D in all three degrees of freedom in a fluid environment. With the help of electro-optic modulators, the properties of the light fields can be changed both quickly and precisely, thus varying the movement direction of the drone. By implementing optical tweezers in the drone body, the drones are capable of transporting and releasing nano-sized cargos like nanodiamonds. Biological applications such as the manipulation of red blood cells, yeast cells or bacterias are also conceivable and are being investigated.

O 71.2 Wed 18:00 Poster D

Plasmonic lightning-rod effect — •Vlastimil Křápek, Rostislav Řepa, Michael Foltýn, Tomáš Šikola, and Michal Horák — Brno University of Technology, Czechia

Field enhancement is one of the key targets in plasmonics [1,2,3]. Intuitively, it is expected that plasmonic antennas (PAs) produce a strong electric field near their sharp features. However, there are other factors besides local curvature contributing to the field enhancement, including the evanescent nature of surface plasmon polaritons or the magnitude of the induced charge for a specific excitation.

In our communication, we isolate the contribution of the local curvature of a PA to the magnitude of the electric field of its dipole plasmon resonance. We design a set of rod-like PAs of identical length with two cylindrical terminations, one with a fixed radius and one with a variable radius. The PAs are investigated by electron energy loss spectroscopy (EELS) and electromagnetic simulations. At the fixed-radius end, we observe the identical loss intensity and field enhancement for all the PAs. This ensures that the variations in the response at the variable-radius end can be attributed purely to the local curvature. Finally, we present an intuitive phenomenological model for the induced electric field based on an effective induced point charge.

[1] M. Hrtoň *et al.*, Phys. Rev. Applied **13**, 054045 (2020).
[2] V. Křápek *et al.*, Nanophotonics **9**, 623 (2020).
[3] O. Bitton *et al.*, Nat. Commun. **11**, 487 (2020).

O 71.3 Wed 18:00 Poster D

Control and measurement of optical fields in a random photonic media — •Diptabrata Paul and Frank Cichos — Peter Debye Institute for Soft Matter Physics, Universität Leipzig, 04103 Leipzig, Germany

The ubiquitous presence of disordered photonic structures in nature has inspired investigation of how wave propagation in complex media could be exploited to control the scattering, transport, and localization of light in matter. However, volumetric scattering in the complex media leads to a universal interference pattern called speckles, which poses a significant challenge in controlling and probing phase and amplitude of light after passing through the medium. To address this, herein, we propose a method by which modulation of incident optical fields using a digital micromirror device (DMD) could achieve modification of optical fields in the random photonic media. Real time imaging of the speckles along with an iterative feedback algorithm sequentially switches the DMD mirror states to on or off positions to achieve incident field binary amplitude modulation and hence desired modification of fields in the medium. On the other hand, we employ a diffuser that could be used for sensing the thermo-optical modulation of an optical field. Specifically, we infer the local perturbation of the wave front by comparing the speckle pattern between a reference and a thermo-optically modified field, which in turn can also quantify the temperature profile. The advent of spatial control over the phase and amplitude of light waves can lead to major advances in fields from imaging and information technology to biomedical optics.

O 71.4 Wed 18:00 Poster D

Programming large-area geometrical phase metasurfaces with the plasmonic phase-change material In_3SbTe_2 — •Florian Bontke[1], Lukas Conrads[1], Andreas Ulm[2], Matthias Wuttig[1], Robert Schmitt[2], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen — [2]Fraunhofer IPT

Phase-change materials (PCMs) have been established as a versatile basis for non-volatile switchable metasurfaces based on a change in the refractive index [1]. Here we employ the novel switchable infrared plasmonic PCM In_3SbTe_2 (IST) whose optical properties can be switched between dielectric (amorphous) and metallic (crystalline) in the full infrared range. While IST has been employed for direct writing of metallic nanoantennas [2] and emissivity shaping metasurfaces [3], its potential for large-area geometric phase metasurfaces remains unexplored. Using circularly polarized light, the geometric Pancharatnam-Berry phase of rotated antennas can be used to obtain full 2π phase control. In this work, a fast commercial laser writing setup is utilized to realize large-area beam steering and other functional metasurfaces for the mid-infrared. Due to the fast writing speed, producing millimeter-scale metasurfaces with over 10^6 individual antennas is feasible. The possibility of creating large-area metasurfaces via direct laser writing without cumbersome fabrication techniques paves the way towards mass production and rapid prototyping of reconfigurable meta-optics in the infrared.

[1] Wuttig et al. *Nat. Photon.* **11**, 465 (2017) [2] Hessler et al. *Nat. Com.* **12**, 924 (2021) [3] Conrads et al. *Adv. Opt. Mat.* **11**, 8 (2023)

O 71.5 Wed 18:00 Poster D

Bloch surface waves on multilayer structures made from tantalum pentoxide and silicon dioxide — •Amélie Wagner and Stefan Linden — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

Bloch surface waves (BSWs) are electromagnetic surface waves that are confined to the interface between a periodic dielectric multilayer structure and a homogeneous dielectric medium. Guiding of BSWs with low propagation losses can be achieved by depositing thin dielectric ridges on top of the multilayer film. BSW waveguides are therefore an attractive alternative to dielectrically loaded surface plasmon polariton waveguides, whose propagation length is limited by Ohmic damping. Here we report on the design and fabrication of BSW waveguides. The multilayer structure consists of alternating tantalum pentoxide (Ta2O5) and silicon dioxide (SiO2) layers deposited by electron beam evaporation. The required thicknesses of the layers are determined beforehand with the help of transfer matrix calculations. In order to test the optical quality of the fabricated samples, we perform total internal reflection measurements in Kretschmann configuration. In the next step, we will deposit dielectric ridges on top of the multilayers by electron beam lithography and evaluate the propagation length by leakage radiation microscopy.

O 71.6 Wed 18:00 Poster D

Scalable 3D Printing of Micro-Optical Elements for Optical Fibres — •Mika Mc Keever and Stefan Linden — Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

3D printing via direct laser writing, utilising two-photon polymerisation has revolutionised the fabrication of micro-optics for optical fibre applications. Previous advancements include the successful printing of optical devices, such as collimating lenses, directly onto the ends of optical fibre. However, the existing technique presents challenges, particularly the manual printing process for each individual fibre, resulting in time-intensive production and difficulties in aligning optical elements with the fibre core. This work addresses these issues by introducing a technique for printing hanging optical elements on a glass substrate, which can be attached to the fibre end. This is achieved by inserting the fibre into a mask that is printed on top. This method

enables the simultaneous printing of multiple optical elements, accelerating production, while maintaining the same printing parameters as direct fibre printing. Moreover, the use of the mask facilitates alignment of the optical elements with the fibre core. By adopting this approach, optical elements with dimensions of up to 300 micrometres can be printed.

O 71.7 Wed 18:00 Poster D

Non-equilibrium electrons generated from the extended two-temperature model to drive chemical dynamics at surfaces — •Henry T. Snowden and Reinhard J. Maurer — University of Warwick, Coventry, UK

A mechanistic understanding of ultrafast light-matter interactions with surfaces and nanoparticles is invaluable for the study of ultrafast dynamics at surfaces. The two-temperature model (2TM) represents the most common approach to model light-matter interaction. It assumes that electrons remain in a Fermi-Dirac distribution, which is heated by a laser source term. This assumption is invalid immediately after a laser pulse, where a short-lived population of non-equilibrium electrons is generated. Here we will explore the extended two-temperature model (e2TM), proposed by Carpene [Phys Rev B 74, 24301 (2006)], including further extensions from Uehlein et al. [Nanomaterials 12, 1655 (2022)]. We will show that the e2TM captures information consistent with simulations based on the Boltzmann transport equation while maintaining much of the simplicity and computational efficiency of the 2TM. We incorporate many parameters directly calculated from first principles, such as the density-of-states (DOS) and properties derived thereof. We present a systematic assessment of the dependence of the e2TM on the type of metal and surface termination and directly relate our results to time-resolved spectroscopy results. Finally, we will examine the necessary properties of a material required to generate long-lived non-equilibrium electrons and suggest possible material candidates.

O 71.8 Wed 18:00 Poster D

Energy and momentum distribution of surface plasmon-induced hot carriers — •Christopher Weiss[1], Tobias Eul[2], Eva Prinz[1], Benjamin Stadtmüller[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern-Landau, Germany — [2]Institute of Experimental and Applied Physics, University of Kiel, Germany

Are the spectroscopic properties of plasmon- and photon-induced carriers fundamentally different? This question is crucial for the advancement of plasmonic energy conversion. Electrons excited at bulk plasmon resonance show a distinct distribution in energy and momentum space [1], while the electron distribution of surface plasmon-induced carriers is still under debate [2].

To address this issue for surface plasmons, we aim to separate the energy and momentum distributions of surface plasmon polariton (SPP)-induced hot electrons from those of photoexcited ones. Exciting a circular ring-slit geometry with radially and azimuthally polarised light, we can clearly separate the plasmon and photon-induced hot carriers in space and time. Our time-resolved photoemission electron microscope (PEEM) is then able to capture their signatures in real time. In this contribution, we show that there are spectroscopic differences between photoemitted electrons and those generated by plasmoemission in the centre of the structure.

[1] Reutzel et al., Phys. Rev. Lett. 123 (2019), 017404
[2] Hartelt et al., ACS Nano 15, 12 (2021), 19559–19569

O 71.9 Wed 18:00 Poster D

Ionization-assisted coherent optical two-dimensional nanoscopy — •Philipp Kessler, Luisa Brenneis, Victor Lisinetskii, Matthias Hensen, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Optical two-dimensional (2D) spectroscopy has proven to be a powerful tool for the investigation of electronic couplings and ultrafast energy transport phenomena. The combination of this technique with photoemission electron microscopy (PEEM), i.e., coherent "2D nanoscopy", enables the investigation of surface system dynamics with high spatio-temporal resolution [1]. However, photoemission may require multiple interactions with individual excitation pulses, causing overlapping signal contributions. The use of an additional ionization pulse circumvents this problem by projecting the population of the system's states into the detection channel via photoemission, as shown in the gas phase [2]. Here, we present modifications of our existing PEEM setup [3] to realize this scheme. This includes second-harmonic generation on a separated beam path to produce the ionization pulse and optimization of the pulse-shaper generated four-pulse excitation sequence, which is accurately reconstructed by spectral interferometry. We further show a new beam stabilization system which enables stable incoupling into the freestanding PEEM by independently stabilizing both beam paths.

[1] M. Aeschlimann et al., Science 333, 1723 (2011).
[2] Uhl et al., Optica 8, 1316 (2021).
[3] Huber et al., Rev. Sci. Instrum. 90, 113103 (2019).

O 71.10 Wed 18:00 Poster D

s-SNOM calibration using multiple tapping harmonics for complex permittivity reconstruction — •Dario Siebenkotten[1], Bernd Kästner[1], Arne Hoehl[1], Manuel Marschall[1], and Shuhei Amakawa[2] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12 10587 Berlin — [2]Graduate School of Advanced Science and Engineering, Hiroshima University, Higashihiroshima, Japan

Infrared scattering-type scanning near-field optical microscopy (s-SNOM) has found wide-spread success in the nanoscale investigation of material properties such as the free-carrier density and crystal structure. The deep sub-wavelength resolution of s-SNOM is achieved by the interaction between the sharp apex of a metallized AFM tip under illumination and the sample surface below it. This complex system poses a difficult inverse problem for the recovery of sample properties from measurements. Recently, a calibration method has been proposed that describes this interaction by means of calibration parameters, instead of fitting the physical characteristics of a heavily idealized tip model [1]. However, the proposed calibration model was designed for a stationary tip, but the use of periodic tip height modulation is essential for s-SNOM measurements. Here, we propose an extension to the model that includes the tip modulation by making use of multiple tapping harmonics. We validate our proposed extension on doped silicon microstructures by reconstructing the permittivity over a broad spectral range and extracting the free-electron density and damping.

[1] Guo et al. Appl. Phys. Lett. 118, 041103 (2021)

O 71.11 Wed 18:00 Poster D

Nano-imaging reveals the stacking dependent dispersion of hybrid polaritons in a Trilayer Graphene and Hexagonal Boron Nitride Heterostructure — •Christian Dittmar, Lina Jäckering, Konstantin Wirth, and Thomas Taubner — I. Institute of Physics, RWTH Aachen University

Two-dimensional (2D) van der Waals (vdW) materials can be combined to heterostructures [1]. Hexagonal Boron Nitride (hBN) and Trilayer Graphene (TLG) are two appealing 2D vdW materials. hBN is a natural hyperbolic material and enables low-loss and volume-confined hyperbolic phonon polaritons (HPhPs) [2]. TLG is gate-tuneable and hosts surface plasmon polaritons. TLG occurs in either a Bernal (ABA) or rhombohedral (ABC) stacking order [3]. Uniting isotopically pure hBN and TLG in a heterostructure enables the formation of hybridized hyperbolic plasmon-phonon polaritons (HP^3). These (HP^3) can be launched and imaged by a scattering-type scanning near-field optical microscope. HP^3 combine the tunability of graphene and the low losses of the HPhPs in hBN. For the first time, we image stacking dependent propagating polaritons in a hBN-TLGN heterostructure. The stacking dependency manifests in the different propagation wavelength originating from different dispersions. The results lay the foundation for distinguishing different stacking orders of TLG encapsulated in hBN and for identifying domain boundaries in TLG. We also emphasize the possibility to image buried structures below an hBN layer.

[1] Basov et al. *Science* **354**, 6309 (2016), [2] Caldwell et al. *Nature Reviews Materials* **4**, 552 (2019), [3] Chen et al. *Nature* **487**, 77 (2012)

O 71.12 Wed 18:00 Poster D

Orientation-dependent interpretation of Janus particle scattering spectra — •Felix Hermann Patzschke, Arthur Markus Anton, and Frank Cichos — Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig

Plasmonic Janus particles consist of dielectric core particles with a thin metallic cap on one side and are widely used in active matter research. The plasmonic cap enhances optical scattering and absorption, allowing for self-propulsion through temperature gradients as well as efficient trapping and tracking. The asymmetry of such a particle gives rise to surface plasmon modes whose excitation is sensitive to the angle at which the particle is illuminated. Even though the angle of illumination strongly influences the particle's scattering response, the

optical properties of such metallic caps have hardly been investigated.

We probe the light scattering of individual micrometre-sized, spherical, Au-coated Janus particles by means of Selective Illumination Multiplexed Fourier Plane Spectroscopy. This novel method allows us to explore microparticles' scattering characteristics resolved for wavelength, angle of illumination and scattering angle. In addition, we supplement our experimental results with finite-element simulations and correlate spectral markers to orientation-dependent surface plasmon modes.

This additional information on the correlation of angular and spectral information could pave the way for new methods of orientation detection. They also shed new light on the interaction of such spherically capped particles with light inducing forces and torques.

O 71.13 Wed 18:00 Poster D

Nanoscale Plasmonic Su-Schrieffer-Heeger Chains — •Benedikt Schurr[1,3], Luisa Brenneis[2], Felix G. Kaps[3,5], Matthias Hensen[2], Philipp Grimm[1,3], Philipp Kessler[2], Tobias Helbig[4], Tobias Hofmann[4], Thorsten Feichtner[1,3], Monika Emmerling[1], Susanne C. Kehr[3,5], Tobias Brixner[2], Ronny Thomale[3,4], Lukas M. Eng[3,5], and Bert Hecht[1,3] — [1]NanoOptics & Biophotonics Group, Experimental Physics 5, University of Wuerzburg — [2]Institut fuer Physikalische und Theoretische Chemie, University of Wuerzburg — [3]Wuerzburg-Dresden Cluster of Excellence ct.qmat — [4]Institute for Theoretical Physics and Astrophysics, 1-4: University of Wuerzburg, Am Hubland, 97074 Wuerzburg, Germany — [5]Institut fuer Angewandte Physik, Technische Universitaet Dresden, 01062 Dresden, Germany

The Su-Schrieffer-Heeger (SSH) model describes one-dimensional (1D) periodic chains of coupled resonators with alternating coupling strengths. It features topologically protected and localized edge states. We fabricate and characterize plasmonic particle SSH-chains with alternating gaps in the nanometer range by focused He-ion beam milling starting from single-crystalline gold micro-platelets. Finite-difference time-domain (FDTD) simulations show the occurrence of edge modes for such geometries whose eigenfrequencies can be controlled by the particle length and the gap size. Using scattering scanning near-field optical microscopy (sSNOM) as well as photoemission electron microscopy (PEEM) of different chain configurations we obtain highly resolved near-field maps indicating edge-state formation.

O 71.14 Wed 18:00 Poster D

Contrast Mechanism Investigation of Single Core-shell Nanoparticles in s-SNOM Using Finite Element Simulations — •Dinghe Dai, Dario Siebenkotten, Richard Ciesielski, and Bernd Kästner — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin

Scattering-type scanning near-field optical microscopy (s-SNOM) is a widely used technique for nanoscale characterization of surface structures, surface polaritons, and biomolecular systems. Recently, core-shell nanoparticles have gained increasing interest in the fields of medical and material sciences. To investigate the properties of single core-shell nanoparticles using s-SNOM, we simulate the near-field contrast characterized by different geometrical and optical properties with the finite element method using the commercial software JCMSuite. We observe different resonances, which shift according to the geometrical properties. Field distribution plots indicate that these resonances may orignate from the interaction between the nanoparticle and the tip as well as between the nanoparticle and the substrate. The simulation results demonstrate the fundamental ability to determine geometrical and optical properties of individual nanoparticles using s-SNOM.

O 71.15 Wed 18:00 Poster D

Improved electron spectrometer for PINEM experiments in an SEM — •Isabella Probst[1], Roy Shiloh[2], Johannes Illmer[1], Franz Schmidt-Kaler[1], and Peter Hommelhoff[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Deutschland — [2]Hebrew University, Jerusalem, Israel

Photon-induced near-field microscopy (PINEM) was demonstrated as a method for imaging electromagnetic fields with femtosecond time resolution. It has developed into intriguing electron light coupling experiments. When electrons interact with an optical nearfield, they can absorb or emit an integer number of photons, modulating the electron spectrum. Most PINEM experiments have been performed in transmission electron microscopes (TEMs). Scanning electron microscopes (SEMs) provide larger sample chambers, are less cost intensive and offer a different range of electron energies. In our SEM-PINEM setup, the electron energy is measured with a custom-built spectrometer [1]. To improve the spectral resolution of our spectrometer, we designed a magnetic lens-based telescope. The performance of the lenses for different positions, coil currents and electron energies was simulated. This improved system will allow investigating a plethora of materials and effects, previously unreachable in an SEM, with improved clarity.

[1] Shiloh, Chlouba, Hommelhoff, PRL 128, 235301 (2022)

O 71.16 Wed 18:00 Poster D

Scattering of controlled plasmonic particles configurations on the mirror — •Aleksei Overchenko and Frank Cichos — Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig

Gold particles have found wide application in sensorics due to their field enhancement propensity that is used for example in Surface-Enhanced Raman Spectroscopy (SERS), Photothermal Therapy and Plasmonic Photovoltaics.

Field enhancement structures can be realised by brining two spheres into proximity, putting a sphere on a mirror or fabricating a bowtie antenna. Surface functionalization often requires complicated modification methods such as lithography and chemical binding, e.g., of DNA origami.

Here, we deliberately manipulate induvial as well as multiple gold particles in front of a gold mirror by local light induced temperature fields generating thermo-osmotic flow fields. We characterize the resulting single, dimeric and higher order clusters, their plasmonic coupling and the coupling of the particles to a thin gold film by scattering spectroscopy. The system is highly reconfigurable as no binding is required and analytes may be bound to the gold film to enable spatially resolved SERS or other field enhancement phenomena.

O 71.17 Wed 18:00 Poster D

Investigation of lithiated carbon as active plasmonic material system — •Valentin Maile, Mario Hentschel, and Harald Giessen — 4th Physics Institute, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Active plasmonic structures are a key component in the recent advances in optical technologies due to their ability to confine and manipulate light on the nano-scale and thus aid the miniaturization of optical devices. A key component for future devices is switchabilty and tunability of the optical resonances. Recently, the electrically switchable metal-to-insulator transition of the organic conjugated polymer PEDOT: PSS was used to realize switchable plasmonic devices at up to 30Hz modulation speed. Here, we introduce a different concept based on lithium-intercalated carbon, a material system known from battery research. The reversible lithium intercalation in the carbon lattice causes an increase of charge carrier density and thus a change in the optical properties of the material, its color changing from black to golden, rendering it an interesting material system for switchable plasmonic nanostructures. In this work, lithiated forms of carbon and their change in optical properties are explored as a possible switchable material system for plasmonic nanostructures. This ansatz expands the toolkit of active plasmonic structures for metasufaces and nanooptics.

O 71.18 Wed 18:00 Poster D

Decoding the Emission from Gold Nanoparticles — •Jan Kutschera, Wouter Koopman, Felix Stete, and Matias Bargheer — University of Potsdam

Surface-enhanced Raman spectroscopy (SERS) has been a valuable tool in biochemical sensing, single-molecule detection, and photocatalysis for several decades. The molecular fingerprints in SERS spectra are always accompanied by a broad background originating from the plasmonic nanoparticles themselves.

In particular, highly clustered nanoparticles, as used in many applications, can produce strong backgrounds. Due to its dependence on the electron distribution of the plasmonic material, understanding this nanoparticle response is crucial for comprehending the mechanisms behind plasmon-enhanced phenomena, such as photochemistry, photovoltaics, and magnetism. While the discussion regarding the underlying processes of this nanoparticle response is ongoing, it is most often attributed to photoluminescence (PL) or electronic Raman scattering (ERS) and thus to intraband processes.

Especially for gold nanoparticles, the contribution of interband transitions must be considered. Utilizing photoluminescence excitation (PLE) spectroscopy, we show the strong dependence on interband excitation, while the emission spectrum continues to be determined by

plasmon-enhanced intraband processes. Furthermore, the presented results support the theory of interband-enabled, Auger-like excitations in the conduction band of gold, followed by intraband emissions in the visible spectrum.

O 71.19 Wed 18:00 Poster D

Automation workflow for ML training on infrared spectra prediction — •Giulio Benedini[1,2], Matti Hellstrom[1], and Luuk Visscher[2] — [1]Software for Chemistry and Materials B.V., De Boelelaan 1083, 1081HV Amsterdam, The Netherlands — [2]Department of Theoretical Chemistry, Vrije Universiteit Amsterdam, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands

Infrared spectroscopy provides information on atomic structure while being cheap and non-invasive technique. Its wide application is hindered by its spectra interpretation. Computational simulations could solve this problem but ab initio approaches have very high computational costs. The use of machine learning interatomic potentials (MLIP) can solve this problem.[1] This work is about workflows to train and assess MLIPs tuned for IR spectra predictions. The FieldSchNet[2] MLIP was used for fitting while workflows were made with PLAMS[3]. The workflow has been developed to favor a re-usable approach. Hyperparameters of FieldSchNet have been optimized with the help of an automated workflow. The training resulted in mean absolute errors for prediction of frequencies of $10cm^{-1}$ and for intensities 7 km/mol on a dataset composed of ethanol and acetaldehyde. Currently active learning scheme needs to be now extend further to include predictions of IR spectra. [1] Chem. Rev. 2021, 121, 16, 10142*10186 [2] Chem. Sci., 2021, 12, 11473 [3] AMS 2023.1, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com.

O 71.20 Wed 18:00 Poster D

Plasmonically induced RAFT polymerization on metal nanoparticles — Pascal Riebler, •Sergio Kogikoski Junior, Matthias Hartlieb, and Ilko Bald — Institute of Chemistry, University of Potsdam, Germany

Reversible addition-fragmentation chain transfer (RAFT) polymerization is one of the most versatile methods to synthesize complex polymeric architectures. This work used plasmonic Ag and Au plasmonic nanoparticles as activation agents instead of standard chemical procedures to generate the radical that will initiate the polymerization. The reactions were done in a usual photochemical setup in solution. Different irradiation wavelengths were used to investigate the activation of the chain transfer agent and the plasmonic nanoparticles. Spectroscopic and microscopic methods extensively characterized the obtained products. SERS results showed that the chain transfer agent used to modify the nanoparticles was detached from the surface to accommodate the newly synthesized polymer. Such a process of detachment generated a surface where monomers could polymerize until the surface coverage was complete, and the charge transfer from the NP to the chain transfer agent was hindered because of the distance. Our systematic results will pave the way for using plasmonic nanoparticles as reliable sources of RAFT-synthesized polymers.

O 71.21 Wed 18:00 Poster D

Hot-electron mediated chirality transfer in single nanoparticles — Seunghoon Lee[1,2], •Chenghao Fan[1], Artur Movsesyan[3], Johannes Bürger[1], Fedja J. Wendisch[1], Leonardo de S. Menezes[1], Stefan A. Maier[1,4], Haoran Ren[4], Tim Liedl[1], Lucas V. Besteiro[5], Alexander O Govorov[3], and Emiliano Cortés[1] — [1]Faculty of Physics, LMU München, 80539 Munich, Germany — [2]Department of Chemistry, Dong-A University, Busan 49315, South Korea — [3]Department of Physics and Astronomy, Ohio University, Ohio 45701, United States — [4]School of Physics and Astronomy, Monash University, Victoria 3800, Australia — [5]CINBIO, University of Vigo, 36310 Vigo, Spain

Recently, chiral plasmonic nanostructures have drawn tremendous interest due to their unique chiroptical properties. Here, we thoroughly investigate the plasmon-assisted growth of chiral nanoparticles from achiral Au nanocubes (AuNCs) via circularly polarized light (CPL) without involvement of any chiral molecules. We identify the structural chirality of our synthesized chiral plasmonic nanostructures by using circular differential scattering (CDS) spectroscopy correlated with scanning electron microscopy imaging at both the single-particle and ensemble levels. Theoretical simulations, including hot-electron surface maps, reveal that the plasmon-induced chirality transfer is mediated by the asymmetric distribution of hot electrons on achiral AuNCs under CPL excitation. Results presented here reveal fundamental aspects of chiral light-matter interaction, influencing the future design and optimization of chiral sensors and chiral catalysis, among others.

O 71.22 Wed 18:00 Poster D

Polarization sensitive plasmonic induced chemical reaction observed by chiral SERS — •Shashank Gahlaut[1], Ki Tae Nam[2], Alexander Govorov[3], and Ilko Bald[1] — [1]Institute of Chemistry, University of Potsdam, Potsdam-14476 Germany — [2]Department of Materials Science and Engineering, Seoul National University, Seoul 08826, S. Korea — [3]Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, Chengdu 610054, China Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701, United States

Plasmonic induced chemical reactions on nanoparticles has attracted the attention of community of material science. Metallic nanoparticles possess the potential of confining the light into sub-wavelength region. The surface plasmon excitation enables the enhancement of local electric field in the close vicinity of particles. The decay of surface plasmons results into the formation of hot charge carriers and localized heat. Solar to chemical energy conversion has become the most attractive application in photocatalysis by plasmonic NPs. Here, we have observed polarization sensitive photochemistry on chemically synthesized chiral plasmonic nanocubes (gold helicoids, AuNC). Dehalogenation of 8-Bromoadenine (8-BrAde), a radiosensitizer, by metallic hot electrons has been targeted as a model chemical reaction. Left-handed AuNC show higher rate of reaction with LCP light as compared to opposite combination of L-AuNC and RCP light. Photochemical g-factor was found to be very large as compare to the optical g-factor. This g factor increases with the increase in laser power.