

MO 24: Large and Reactive Systems

Time: Friday 10:30–12:30

Location: S HS 002 Biologie

MO 24.1 Fri 10:30 S HS 002 Biologie
Effectiveness of Dye Sensitized Solar Cells (DSSCs) based on Cu-doped TiO₂ photoanodes. — ●SARA CHAHID — SCEM research group, Department of Physical Chemistry, Faculty of Sciences, University of Cádiz, 11510, Puerto Real (Cádiz), Spain.

In this research, Cu-doped TiO₂ nanostructures with different doping contents from 0 to 10.0% (mole fraction) were synthesized through hydrolysis at low temperature. The as-prepared Cu-doped TiO₂ nanostructures was characterized with several techniques, X-ray diffraction (XRD) and Raman spectroscopy were used to study the morphology and structure of the nanoparticles, which confirmed the crystalline anatase tetragonal structure. The UV-Vis Spectroscopy analysis was found that incorporation of Cu²⁺ into titanium affects the band gap of TiO₂ and extending his activity towards visible sunlight region. Scanning Electron Microscopic (SEM) analysis confirming the Cu content is incorporated into TiO₂ lattice affecting efficiency of doped samples. Further, the active specific surface area of the system was investigated employing Brunauer-Emmet-Teller (BET) measurement. Then the Dye-sensitized solar cells (DSSCs) based on Cu-doped TiO₂ photoanodes were fabricated and investigated with chemically adsorbed Ruthenium N3 dye electrode under light illumination with standard solar simulator (AM 1.5G, 100mW/cm²). Results demonstrated that the 1.0% Cu-doped TiO₂ sample annealed at 773K for 60 minutes exhibited the best photovoltaic performance of open circuit voltage ($V_{oc} = 957.5$ mV), short circuit current density ($J_{sc} = 0.795$ mAcm⁻²), and the cell efficiency was reached ($\eta = 4.524\%$), which consists 50% higher than the un-doped cell. This study may open up more investigated works applying Cu doped TiO₂ in photovoltaic fields.

MO 24.2 Fri 10:45 S HS 002 Biologie
Synthesis of cubic tin sulfide nanocrystals: growth mechanism unfolded by organic ligands adsorption — ●ELAD SEGEV^{1,2}, RAN EITAN ABUTBUL^{1,2}, URI ARGAMAN¹, YUVAL GOLAN^{1,2}, and GUY MAKOV^{1,2} — ¹Department of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel — ²Ilse Katz institute for Nanoscale science and Technology, Ben-Gurion University of the Negev, Beer-Sheva 84105m Israel

Novel metastable cubic phase was recently discovered in tin monosulfide and monoselenide systems. Surface energy calculations and experimental studies indicate that this cubic phase is stabilized by specific ligands adsorption on the surface. In this work, it is shown experimentally that HCl molecule, which incorporated to the reaction medium as Oleylammonium chloride (OACl) salt, stabilized those novel phases. The ab-initio computations with adsorbed ligands show lower surface energies for the cubic phase and for the orthorhombic phase than for the pristine surfaces. It is shown that Cl bonds are replacing the missing Sn-S bonds on the surface in the cubic structure. We show that high ligand concentration reaching a full surface coverage enables the cubic nanoparticles to stabilize while for the same concentration the orthorhombic nanoparticles collapse.

MO 24.3 Fri 11:00 S HS 002 Biologie
Fate of inorganic and organic P-compounds: new insights from quantum-chemical modelling — ●ASHOUR AHMED and OLIVER KÜHN — Institute of Physics, University of Rostock, Rostock, Germany

Facing the projected peak phosphorus (P) scenario, substantial research activities have been triggered to improve our knowledge towards a more efficient and sustainable use of P resources. One major factor playing a role in the P immobilization is its strong interaction with soil mineral surfaces and especially with Fe- and Al-oxides. A systematic molecular-level picture of the P binding mechanism at mineral surfaces is still lacking. Therefore, our main target is to explore the molecular binding mechanism for the P adsorption at mineral surfaces in the presence of water. The current presentation is focusing on simulation the binding of different organic and inorganic P compounds with the goethite (α -FeOOH) and its isomorphous (diaspore, α -AlOOH) mineral surfaces. Here, periodic DFT MD simulations are applied to explore possible binding mechanisms for these P compounds at different surface planes. The simulation results indicated to covalent bond formation between P and the mineral surfaces with several binding motifs. These interactions are accompanied by formation of H-bonds,

proton transfer, and water dissociation at the mineral surface. More results will be introduced through our presentation at the conference. References 1. Kruse et al., Journal of Plant Nutrition and Soil Science 178, 43 (2015) 2. Ahmed et al., Physical Chemistry Chemical Physics 20, 1531 (2018)

MO 24.4 Fri 11:15 S HS 002 Biologie
Transient absorption spectroscopy of nanodiamonds in water: direct observation of solvated electrons — ●CHRISTOPH MERSCHJANN¹, FRANZISKA BUCHNER¹, BENJAMIN KIENDL², AMÉLIE VENEROSY³, HUGUES GIRARD³, JEAN-CHARLES ARNAULT³, EMINA HADZIFEJZOVIC⁴, JOHN FOORD⁴, ANKE KRUEGER², and TRISTAN PETIT¹ — ¹Helmholtz-Zentrum Berlin, Germany — ²Universität Würzburg, Germany — ³CEA-LIST, Saclay, France — ⁴University of Oxford, United Kingdom

Nanodiamonds (ND) are promising candidates for photocatalytic transformation of CO₂ to CO and organic reduction products like methanol or formic acid, as they release solvated electrons to the aqueous solution upon UV illumination. However, the nature of the electron emission process and its related dynamics are still unknown.

We investigate the ultrafast dynamics of this process using femtosecond transient absorption spectroscopy with DUV (225 nm) pump and VIS supercontinuum probe pulses. While the recombination of solvated electrons is governed by long-lived (> 2 ns) diffusion processes, NDs of different surface termination (-H, -OH, -COOH) show characteristic features in the sub-picosecond regime. We will discuss the impact of these surface terminations on the dynamics of solvated electrons, and thus on the photocatalytic performance in water. We expect that our results will support the design of efficient metal-free photocatalysts for CO₂ conversion.

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MO 24.5 Fri 11:30 S HS 002 Biologie
Joining Microfluidics with Infrared Photodissociation: Shedding Light on ortho-Quinone Methides, a Highly Reactive and Transient Intermediate — ●MARTIN MAYER, MAX GRELLMANN, and KNUT R. ASMS — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstrasse 2, D-04103 Leipzig, Germany

Chemical microreactors, such as microfluidic chips, are revolutionizing the way we can study chemical reactions by making time scales available that were not reachable with conventional techniques. Here, we combine microfluidic chips with the structure determining power of infrared photodissociation (IRPD) spectroscopy to shed light on the in-situ formation of ortho-quinone methides (o-QM). Those highly reactive, transient and therefore not isolatable intermediates occur in innumerable natural processes and have a huge potential in organic synthesis, especially regarding stereoselective reactions. The ephemerality of o-QMs often prevents their investigation by conventional analytical methods. By coupling microfluidics with IRPD spectroscopy, we are not only able to characterize the structures, but also determine E/Z ratios of o-QMs which are produced in-situ on chip. This information is given by the analysis of the IR fingerprint regions of the short-lived species. Control over stereoselectivity is achieved by introducing lewis acidic alkali metal ions into the reactions and monitoring stereoisomer-selective IR absorption bands which reflect the resulting E/Z ratio. With this multidimensional approach we are able to gain a deeper understanding and control over the formation of elusive o-QMs.

MO 24.6 Fri 11:45 S HS 002 Biologie
Infrared Emission from Thermally Excited Strongly Coupled Vibrational Transitions — ●MARCUS SEIDEL, ANOOP THOMAS, THIBAUT CHERVY, KALAIVANAN NAGARAJAN, ELOISE DEVAUX, CYRILAQUE GENET, and THOMAS W. EBBESEN — ISIS & icFRC, University of Strasbourg, CNRS, 67000 Strasbourg, France

The strong coupling of vibrational transitions to microcavity resonances has shown a decisive impact on chemical reactivity and likewise presents an exciting platform for studying quantum effects related to the light-matter hybridized quasi-particles, called vibro-polaritons [1,2]. Recently, first data was obtained from vibro-polariton thermal

emission [3]. Here, we significantly extend this initial work. We present temperature and cavity tuning dependent emission measurements from strongly coupled liquids, namely diethyl sebacate and tetrachloroethylene. This results in better cavity tunability and an increased range of polariton excitation densities. Furthermore, we complement the experimental method by normal incidence reflection measurements and by employing microcavities with dielectric mirrors. The performed experiments lead to a reinterpretation of the previously reported results. In particular, we show that the investigated vibro-polaritonic states are thermalized and that polariton-polariton interactions cannot be readily extracted from the emission data. Our results are important for pioneering vibro-polariton interactions which are crucial for condensation of the quasi-particles. References: [1] T. W. Ebbesen, *Acc. Chem. Res.* 49, 2403 (2016). [2] D. S. Dovzhenko et al., *Nanoscale* 10, 3589 (2018). [3] T. Chervy et al., *ACS Photon.* 5, 217 (2018).

MO 24.7 Fri 12:00 S HS 002 Biologie

Can you hear an axon growing? — ●FREDERIC FOLZ¹, LUKAS WETTMANN¹, GIOVANNA MORIGI¹, and KARSTEN KRUSE² — ¹Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany — ²NCCR Chemical Biology, Departments of Biochemistry and Theoretical Physics, University of Geneva, 1211 Geneva, Switzerland

Axons are linear structures of nerve cells that can range from a few tens of micrometers up to meters in length. In addition to external cues, the length of an axon is also regulated by unknown internal mechanisms. Molecular motors have been suggested to generate oscillations with an axon-length dependent frequency that could be used to measure an axon's extension. Here, we present a mechanism for determining the

axon length that couples the mechanical properties of an axon to the spectral decomposition of the oscillatory signal.

MO 24.8 Fri 12:15 S HS 002 Biologie

Diagrammatic Monte Carlo approach to angular momentum in quantum many-body systems — ●GIACOMO BIGHIN¹, TIMUR TSCHERBUL², and MIKHAIL LEMESHKO¹ — ¹IST Austria (Institute of Science and Technology Austria), Am Campus 1, 3400 Klosterneuburg, Austria — ²Department of Physics, University of Nevada, Reno, NV, 89557, USA

We introduce a Diagrammatic Monte Carlo (DiagMC) approach to molecular impurities, possessing rotational degrees of freedom [1]. The technique is based on a diagrammatic expansion [2] that merges the usual Feynman diagrams with the angular momentum diagrams known from atomic and nuclear structure theory, thereby incorporating the non-Abelian algebra inherent to quantum rotations. Due to the peculiar way in which angular momenta couple, the configuration space is larger with respect to most DiagMC applications, and a new class of updates is needed in order to span it completely.

We exemplify the technique by obtaining an all-coupling solution of the angulon model - essentially a molecular impurity in a quantum many-body environment - showing that our approach correctly recovers the strong-coupling limit. However, the technique is general and can be applied to a broad variety of systems possessing angular momentum degrees of freedom, thereby establishing a far-reaching connection between DiagMC techniques and molecular simulations.

[1] G. Bighin, T. V. Tscherebul, and M. Lemeshko, *Phys. Rev. Lett.* 121, 165301 (2018). [2] G. Bighin and M. Lemeshko, *Phys. Rev. B* 96, 419 (2017).