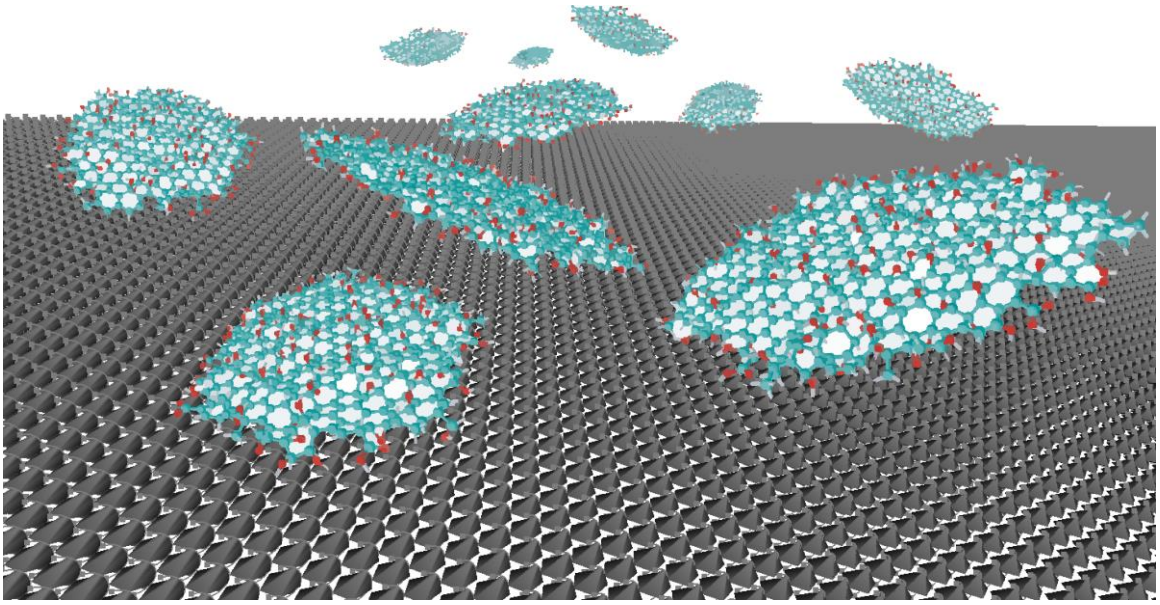
4th Erwin Schrödinger Symposium 2021

of the Erwin Schrödinger Society for Nanosciences

„Advanced Materials“



January 11 - 12, 2021

Online

1st day: https://zoom.us/j/92815377029?pwd=V3NpcUF4ZGdxQmRNWHFyZmp1SElwUT09

2nd day: https://zoom.us/j/96938446312?pwd=SzRBUWM4bkc4SWEyZm42U2o3SmdOQT09

http://www.esg-nano.ac.at/

Chair: Wolfgang Kautek

Organization committee: Oskar Armbruster, Eva Ehmoser, Wolfgang Kautek, Aida Naghilou

Foreword

The **4th Erwin Schrödinger Symposium 2021** of the Erwin Schrödinger Society for Nanosciences **“Advanced materials”** is intending to instill vivid scientific communication and discussion in synthetic, biogenetic, and biomimetic Advanced Materials in respect to their fabrication methods, characterization properties, size effects, applications, and modelling for relating features and structures.

This symposium is organized by the Erwin Schrödinger Society for Nanosciences in a series of successful predecessor events, the **1st Erwin Schrödinger Symposium 2014 “Two Dimensional Nanostructures”** (November 2014, Vienna, Austria), the **2nd Erwin Schrödinger Symposium 2016 “Zero Dimensional Nanostructures: Science and Technology of Nanoparticles”** (May 2016, Vienna, Austria), and the **3rd Erwin Schrödinger Symposium 2018 „Progress in Interfacial Nanosciences“** (June 2018, Dornbirn, Austria).

International experts will illustrate the importance of Advanced Materials in future applications. The conference features active discussions in oral sessions.

Vienna, January 2021

Wolfgang Kautek
(Chair of the 4th Erwin Schrödinger Symposium 2021
& Vice President of the Erwin Schrödinger Society for Nanosciences)

Organizer

Erwin Schrödinger Society for Nanosciences
University of Natural Resources and Life Sciences, Vienna
Institute for Synthetic Bioarchitectures
Muthgasse 11/II
A-1190 Vienna, Austria
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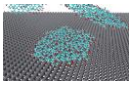
Federal Ministry
Republic of Austria
Climate Action, Environment,
Energy, Mobility,
Innovation and Technology

NanoSyn



Program

Monday, January 11, 2021 (Morning)

09:00 – 09:30 **Welcome**

09:30 – 10:00 **Lecture 1:**
Olav Galteland
Norwegian University of Science and Technology, NO
Pressures of nanosized systems described by Hill's thermodynamics of small systems

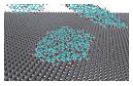
10:00 – 10:30 **Lecture 2**
Piero Baglioni
University of Florence, IT
New methods and materials for the conservation of Cultural Heritage: from renaissance frescoes to modern and contemporary art

10:30 – 11:00 **Coffee Break**

11:00 – 11:30 **Lecture 3**
Sefik Suzer
Bilkent University, TR
Operando-XPS Investigation of Electrified Solid/Liquid Interfaces using Lab-Based Instruments for Energy Storage Systems

11:30 – 12:00 **Lecture 4**
Katharina Al-Shamery
Carl von Ossietzky University of Oldenburg, DE
Understanding heterogeneous Catalysis fundamentally: From Single Site Reactions to Nanstructured Systems

12:00 – 13:00 **Lunch Break**



Monday, January 11, 2021 (Afternoon)

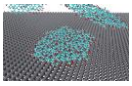
13:00 – 13:30 **Lecture 5**
Ille C. Gebeshuber
TU Wien, AT
Biomimetic and bio-inspired advanced materials

13:30 – 14:00 **Lecture 6**
Magdalena Parlinska-Wojtan
Polish Academy of Sciences, PL
Fancy nanomaterials for fancy applications

14:00 – 14:30 **Coffee Break**

14:30 – 15:00 **Lecture 7**
Eckart Rühl
Free University of Berlin, DE
Nanoparticles in Fundamental and Applied Research

15:00 – 15:30 **Lecture 8**
Venkata Sai Avvaru
IMDEA Materials Institute, ES
High energy/power density lithium-ion batteries through interface engineered CoO@3D-NRGO pseudocapacitive anodes



Tuesday, January 12, 2021 (Morning)

09:00 – 09:30 **Lecture 9**
Israt Ali
Chinese Academy of Sciences, CN
Humidity responsive Polymer/Gold nanoparticles based hybrid Aerogel for real time Monitoring of Human breath

09:30 – 10:00 **Lecture 10**
Oliver Gröning
Swiss Federal Laboratories for Materials Science and Technology, CH
Engineering of electronic and magnetic properties in all carbon nanostructures

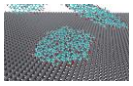
10:00 – 10:30 **Lecture 11**
Peter Ertl
TU Wien, AT
Lab-on-a-Chip Systems in Precision Medicine and Personalized Diagnostics

10:30 – 11:00 **Coffee Break**

11:00 – 11:30 **Lecture 12**
Thomas Bürgi
University of Geneva, CH
Thiolate-protected metal clusters: Chirality and dynamic nature

11:30 – 12:00 **Lecture 13**
Alexander M. Bürger
TU Wien, AT
Antibacterial Surface Structures of Cicada Wings and Technical Replication

12:00 – 13:00 **Lunch Break**



Tuesday, January 12, 2021 (Afternoon)

13:00 – 13:30 **Lecture 14**
Alexander Pogany
Federal Ministry for Climate Action, Environment, Energy, Mobility, Innovation and Technology, AT
Austrian R&D-Policy in Nantechnology

13:30 – 14:00 **Lecture 15**
Mewin Vincent
IMDEA Materials Institute, ES
Investigation of dual-phase TiO_2 nanosheet as pseudocapacitive cathodes for Long lasting Mg-Li hybrid batteries

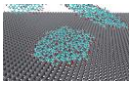
14:00 – 14:30 **Lecture 16**
Antreas Afantitis
NovaMechanics Ltd, CY
NanoSolveIT: Nanoinformatics Hazard, EcoTox and Exposure Models

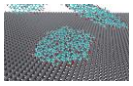
14:30 – 15:00 **Coffee Break**

15:00 – 15:30 **Lecture 17**
Aida Naghilou
Medical University of Vienna, AT
Spider Silk: A nature given template for an advanced material

15:30 – 16:00 **Lecture 18**
Shuguang Zhang
Massachusetts Institute of Technology, US
QTY code: A simple tool for designs of water-soluble membrane protein, unexpected discovery of truncated receptors that retain biological functions

16:00 – 16:30 **Summary**





Lectures

Federal Ministry
Republic of Austria
Climate Action, Environment,
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NanoSyn

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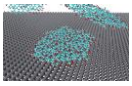


Lecture 1

Pressures of nanosized systems described by Hill’s thermodynamics of small systems

Olav Galteland, Michael T. Rauter, Máté Erdős, Signe Kjelstrup, Dick Bedeaux, Sondre K. Schnell, Thijs J. H. Vlugt, Othonas A. Moultos

PoreLab, Norwegian University of Science and Technology
Engineering Thermodynamics, Process & Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, DelftUniversity of Technology
Department of Materials Science and Engineering, Norwegian University of Science and Technology

The Gibbs equation is not Euler homogeneous of the first order for small systems. A consequence of this is that the common thermodynamic machinery can not be applied to small systems. Hill generalized the Gibbs equation to be Euler homogeneous of the first order for all systems [1], this new equation has been called the Hill-Gibbs equation. For large systems the Hill-Gibbs equation reduces to the Gibbs equation. The Hill-Gibbs equation describes the thermodynamic state of an ensemble of N small systems, where N is the new thermodynamic independent variable that makes the Hill-Gibbs equation Euler homogeneous of the first order. The conjugate variable of N is the sub-division potential ε, which describes the change in the total internal energy when another small system is added to the ensemble while keeping the total entropy, number of particles, volume and shape constant. A consequence of the new thermodynamic variable N is that there are two different pressures for small systems, the differential and integral pressure. The term small systems is general, and the Hill-Gibbs equation can be applied to for example zeolites, metal-organic frameworks, droplets, etc.

In this work we have investigated two model systems, a slit and a cylindrical nanopore filled with fluids [2, 3]. We have applied Monte Carlo and molecular dynamic simulations to study these systems. A central question in this work is how the new thermodynamic variables can be interpreted in terms of the mechanical pressure tensor as computed in molecular simulations. For a liquid droplet in a slit pore we show that the tangential pressure tensor component is equal to the integral pressure and the normal pressure tensor component is equal to the differential pressure. The integral pressure is equal along the pore in equilibrium, while the normal pressure is different in the liquid and the vapor for contact angles not equal to 90°.

The difference in the normal pressure is described by the Young-Laplace equation. For slit pores with a distances between the parallel plates smaller than 3 nanometers, there is a strong force between the parallel plates, this force is the disjoining force. We show how the disjoining pressure can be described by using Hill’s thermodynamics of small systems.

[1] T. L. Hill, “Thermodynamics of Small Systems,” New York: Dover, 1964.
[2] M. T. Rauter, O. Galteland, S. K. Schnell, D. Bedeaux, and S. Kjelstrup, “Equilibrium Pressures in Hydrophobic Pores,” pp. 1–22.
[3] M. Erdős, O. Galteland, D. Bedeaux, S. Kjelstrup, O. A. Moultos, and T. J. Vlugt, “Gibbs ensemble monte carlo simulation of fluids in confinement: Relation between the differential and integralpressures,” Nanomaterials, vol. 10, no. 2, 2020.

Lecture 2

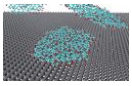
New methods and materials for the conservation of Cultural Heritage: from renaissance frescoes to modern and contemporary art

Piero Baglioni

Department of Chemistry and CSGI, University of Florence

We pioneered one of the most exotic application of soft matter and materials science to conservation of cultural heritage. Art Conservation poses a formidable and exciting challenge to soft matter-colloid scientists in two respects. First, the majority of the most performing and environmentally safe cleaning and consolidation agents for artworks are soft matter systems. Second, the interaction of these agents with the artifact involves an exceptionally complicated range of interfacial interactions. Works of art surfaces interacting with the environment are the most prone to aging and decay; accordingly, soiling is a prime factor in the degradation of surfaces, chemical and mechanical degradation are often associated to soiling and lead to the disfigurement of a piece of art. The effects of these processes are usually strongly amplified in the presence of protective coatings (mainly acrylic and vinyl polymers), applied in previous restoration treatments. We pioneered the synthesis and the application of several advanced systems for the consolidation and the cleaning of works of art, as hydroxides nanoparticles, microemulsions and chemical gels. These systems mark a paradigm shift in modern conservation and have been used on classic, modern and contemporary artifacts as wall paintings of Beato Angelico, Piero della Francesca, or on modern and contemporary art paintings as paintings by Picasso, Lichtenstein, Pollock, de Chirico, etc.. I will summarize the main progresses and perspectives that this field can disclose to Chemists and Conservators communities.

[1] Mastrangelo, R, Chelazzi, D., Poggi, G., Fratini, E., Buemi, LP., Petruzzellis, ML., Baglioni, P. - Twin-chain polymer hydrogels based on poly(vinyl alcohol) as new advanced tool for the cleaning of modern and contemporary art. PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA 2020, 117, 7011-7023. DOI: 10.1073/pnas.2011246117
[2] Montis, C.; Koynov, K.; Best, A.; Baglioni, M.; Butt, H-J.; Berti, D.; Baglioni, P. - Surfactants Mediate the Dewetting of Acrylic Polymer Films Commonly Applied to Works of Art. ACS Applied Materials & Interfaces 2019, 11, 27288-27296.
[3] Bonelli, N.; Montis, C.; Mirabile, A.; Berti, D.; Baglioni, P. - Restoration of paper artworks with microemulsions confined in hydrogels for safe and efficient removal of adhesive tapes. PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA 2018, 115, 5932-5937
[4] Baglioni, Michele, Montis, Costanza, Chelazzi, David, Giorgi, Rodorico, Berti, Debora, Baglioni, Piero (2018). Polymer Film Dewetting by Water/Surfactant/Good-Solvent Mixtures: A Mechanistic Insight and Its Implications for the Conservation of Cultural Heritage. ANGEWANDTE CHEMIE. INTERNATIONAL EDITION, vol. 57, p. 1-6, ISSN: 1433-7851, doi: 10.1002/anie.201710930
[5] Baglioni, M., Montis, C., Brandi, F., Guaragnone, T., Meazzini, I., Baglioni, P., Berti, D. (2017). Dewetting acrylic polymer films with water/propylene carbonate/surfactant mixtures - Implications for cultural heritage conservation. PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol. 19, p. 23723-23732, ISSN: 1463-9076, doi: 10.1039/c7cp02608k
[6] Raudino, Martina, Giamblanco, Nicoletta, Montis, Costanza, Berti, Debora, Marletta, Giovanni, Baglioni, Piero (2017). Probing the Cleaning of Polymeric Coatings by Nanostructured Fluids: A QCM-D Study. LANGMUIR, vol. 33, p. 5675-5684, ISSN: 0743-7463, doi: 10.1021/acs.langmuir.7b00968
[7] Mastrangelo, Rosangela, Montis, Costanza, Bonelli, Nicole, Tempesti, Paolo, Baglioni, Piero (2017). Surface cleaning of artworks: Structure and dynamics of nanostructured fluids confined in polymeric hydrogel networks. PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol. 19, p. 23762-23772, ISSN: 1463-9076, doi: 10.1039/c7cp02662e
[8] Baglioni Piero, Carretti Emiliano, Chelazzi David (2015). Nanomaterials in art conservation. NATURE NANOTECHNOLOGY, vol. 10, p. 287-290, ISSN: 1748-3387, doi: 10.1038/nnano.2015.38



Lecture 3

Operando-XPS Investigation of Electrified Solid/Liquid Interfaces using Lab-Based Instruments for Energy Storage Systems

Sefik Suzer

Department of Chemistry, Bilkent University, 06800 Ankara, Turkey

X-Ray based Operando Investigations have traditionally been carried out in Synchrotron facilities, due to demanding instrumentation and expertise.1, 2 However, although sporadic, several important lab-based XPS studies have also been reported.3 Emergence of Ionic Liquids with several promising properties, including their low volatility, has rekindled the use of XPS, especially for Operando types of measurements.4 Our initial investigations had also concentrated on ionic-liquids and their interfaces under dc and ac electrical bias, and extended to monitoring electrochemical reactions.5, 6 Recently, we have been investigating other low-volatile liquids and their drops on various substrates to tap into the Electrowetting phenomena.7-9 The common theme in all of our studies is the use of bias dependent shifts in the positions of the core-levels as reflection of the electrical potentials, recorded in a totally non-invasive and chemically resolved fashion. We use the magnitude and the frequency dependence of such potentials to extract pertinent information related to static, as well as dynamic chemical and/or electrochemical properties of the materials and their interfaces.10 Examples using ionic liquids, liquid poly-ethylene-glycol (PEG) and their mixtures, with special emphases on energy storage systems, will be presented and discussed.

[1] Bluhm, H.; Andersson, K.; Araki, T.; Benzerara, K.; Brown, G. E.; Dynes, J. J.; Ghosal, S.; Gilles, M. K.; Hansen, H.-C.; Hemminger, J., J. Electron Spectrosc. Relat. Phenom. 150, 86-104 (2006).
[2] Lichterman, M. F., Hu, S., Richter, M. H., Crumlin, E. J., Axnanda, S., Favaro, M., Drisdell, W., Hussain, Z., Mayer, T., Brunschwig, B. S., Lewis, N. S., Liu, Z. & Lewerenz, H.-J. Energy & Environmental Science 8, 2409-2416 (2015).
[3] Foelske-Schmitz; A., Ruch; P.W., Kötz; R., J. Electron Spectrosc. Relat. Phenom. 182, 57-62 (2010).
[4] Lovelock, K. R. J., Villar-Garcia, I. J., Maier, F., Steinrück, H.-P. & Licence, P.. Chemical Reviews 110, 5158-5190, (2010).
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[7] Gokturk P.A.; Ulgut; B.; Suzer; S., Langmuir 34, 7301-7308 (2018).
[8] Gokturk, P.A.; Ulgut; B.; Suzer; S., Langmuir 35, 3319-3326 (2019).
[9] Uzundal, C.B., Ozgur, S.; Aydogan-Gokturk, P.; Wu, H.; Mugele, F.; Ulgut, B.; Suzer, S., Langmuir 35, 16989−16999 (2019).
[10] Uzundal, C.B.; Aydogan-Gokturk, P.; Suzer, S.; Ulgut, B., J. Phys. Chem. C 123, 13192-13200 (2019).

Lecture 4

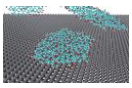
Understanding heterogeneous Catalysis fundamentally: From Single Site Reactions to Nanstructured Systems

Katharina Al-Shamery

Carl von Ossietzky University Oldenburg, Institute for Chemistry, D-26111 Oldenburg, Germany

Heterogeneous Catalysis plays a key role in chemical industry to lower activation barriers in chemical production. The catalysts are normally complex hybrid systems, often consisting of metal nanoparticles on oxidic supports. Catalytic reactions may involve a large number of elementary steps. However, in order to tailor the catalyst to the need of a specific chemical reaction it is essential to understand a multitude of different aspects. Single defects and dopants at the oxidic support may be responsible for the population of various reaction paths. In case of the use of metal nanoparticle cocatalysts, the size, composition and structure of the nanoparticle, as well as the interaction between the particle and the support may be essential. Molecules adsorbed at the nanoparticles may act as reactants, poisons or spectators. Ultra High Vacuum (UHV) techniques are useful to study single molecule surface interactions to get an insight into the most important elementary steps. In the talk the relevance of different Ti3+/Ti4+ ratios in a TiO2(110) single crystal will be demonstrated as an example to influence partial oxidation, deoxygenation or C-C-coupling reactions of alcohols and aldehydes [1]. In order to study the interaction of metal nanoparticle cocatalysts a colloidal approach will be presented allowing to control the size, shape, particle loading and the study of the nanoparticle support interaction in contrast to classical impregnation-calcination techniques. The ligands stabilizing the colloids may further influence the selectivity of the chemical reaction [2]. The talk will focus on amine capped platinum and alloy nanoparticles [3].

[1] Milena Osmić, Lars Mohrhusen, Katharina Al-Shamery J. Phys. Chem. C, 123 (2019), 7615-7626, DOI: 10.1021/acs.jpcc.8b02953
[2] Michael Siemer, Gabriele Tomaschun, Thorsten Klüner, Philipp Christopher, Katharina Al-Shamery ACS Applied Materials & Interfaces, 12 (2020) 27765-27776
[3] L. Altmann, XD Wang, J. Stöver, M. Klink, V. Zielasek, K. Thiel, J. Kolny-Olesiak, K. Al-Shamery, H. Borchert, J. Parisi, M. Bäumer, ChemCatChem, 5 (2013) 1803-1810.



Lecture 5

Biomimetic and bio-inspired advanced materials

Ille C. Gebeshuber[1], Gloria Rose[2], Anna Pavlicek[2], André Gazsó[2]

[1] Vienna University of Technology
[2] Austrian Academy of Sciences

This invited lecture explores bio-inspired and biomimetic nanomaterials, differentiating between bio-inspired or biomimetic nanotechnology and bio-nanotechnology. Following a clarification of these terms, the basics of bio-inspired and biomimetic nanomaterials are presented. Subsequently, a systematic classification of synthetic methods of bio-in- spired and biomimetic nanomaterials is given, based on the method of manufacturing and not on the functionality of the materials. This enables a more coherent correlation with safety aspects, which are yet to be defined in many cases. Due to the great variety, a categorization according to material properties or material compositions is not considered practical. In addition to chemical properties, physical parameters such as size, structure and surface quality play an important role in the categorization. In summary, it can be said that bio-inspired and biomimetic nanomaterials represent important base materials as so-called functional advanced materials in research, development and industry – provided that the material development is accompanied by a corresponding safety and sustainability-oriented technology assessment.

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Lecture 6

Fancy nanomaterials for fancy applications

Elżbieta Drzymała[1], Aleksandra Indyk[1,2], Joanna Depciuch[1], Bartosz Klębowski, Magdalena Laskowska[1], Magdalena Parlinska-Wojtan[1]

[1] Institute of Nuclear Physics, Polish Academy of Science, ul. Radzikowskiego 152, 31-342 Kraków, Poland
[2] Rzeszow University of Technology, al. Powstańców Warszawy 12, 35-959 Rzeszów, Poland

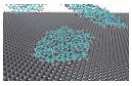
Fancy-shaped nanoparticles as well as multicompoent nanostructures were synthesized and tested for biomedical and fuel cell applications. Noble metal nanoparticles (NPs), are known as sensitizers able to increase the therapeutic effect of photothermal or proton irradiation therapy of cancer cells. Au NPs are excellent photothermal sensitizers – we synthesized differently shaped Au NPs: spherical, rod-like, porous, nanopeanuts and nanodahlias (NDs) [1], which have a very developed surface due to the presence of petal-like structures. The NDs were added to colon cancer cell lines (SW480 and SW620) and laser irradiated with different electromagnetic wavelengths (405 nm, 650 nm and 808 nm) reaching 50 % photothermal conversion efficiency.

To increase the effectiveness of proton beam irradiation of cancer cells, crystalline, 60 nm AuPt nanocauliflowers (NCs) were synthesized using green chemistry method [2]. The NCs were placed into cell culture of colon cancer cell lines (HCT116, SW480 and SW620) and normal colon cell line (FHC), and subsequently subjected to proton irradiation with a total dose of 15 Gy. The MTS viability test, performed after 18 h incubation of the irradiated cell culture with AuPt NCs, showed a significantly higher mortality of cancer cells compared to the normal cells.

Carbon supported nanostructured platinum and platinum-based systems are commonly used as electrocatalysts for ethanol oxidation reaction (EOR), but are not the optimal anodic catalyst for direct ethanol fuel cells. We synthesized ternary Pt/Re/SnO_2/C catalysts, which showed several times higher electrocatalytic activity towards EOR compared to commercial Pt [3]. In order to increase the active surface of the catalytic nanoparticles, hollow, rhombic dodecahedron PtRhNi nanoframes were synthesized and subsequently decorated with SnO_2 NPs. Their specific activity for EOR was ten times higher compared to commercial Pt [4]. Currently, we are designing and developing Pt-free catalysts for EOR. Cerium oxide and metallic palladium nanocubes (NCs) were synthesized separately. Subsequently, the Pd NCs were deposited on the larger and porous CeO_2 NPs. The Pd@CeO_2/C catalysts perform much better for EOR compared to pure Pd NCs.

[1] J. Depciuch et al. J. Mat. Sci., 55 (2020) 2530
[2] B. Klebowski et al. Int. J. Mol. Sci. 21(24) (2020) 9610
[3] E. Drzymała et al. Nano Research, 13(3) (2020) 832
[4] G. Gruzeł et al. ACS Appl. Mater. Interfaces, 112 (2019) 2352

Financial support from the Polish National Science Centre (NCN), grant UMO-2019/35/B/ST5/04140 is acknowledged.



Lecture 7

Nanoparticles in Fundamental and Applied Research

Eckart Rühl

Institute of Chemistry and Biochemistry, Free University of Berlin

Local probing of nanoscopic matter by spectroscopy and spectromicroscopy is reviewed. Targets are free nanoparticles in the gas phase, nanoscopic matter in liquid microdroplets, deposited nanosystems, and nanoscopic matter in biological surroundings. The experimental studies are primarily performed by tunable soft X-rays, in the infrared regime, as well as complimentary radiation sources, including free electron lasers and laboratory-based short pulse lasers.
Properties of free nanoparticles prepared in a narrow beam are investigated by soft X-rays. This approach has the advantage that single particles without any contact to a substrate are probed so that radiation damage and charging effects are efficiently suppressed. The emission of electrons or ions is probed as a function of photon energy. Light scattering and photoemission studies reveal distinct information on the surface structure and composition of nanoparticles [1, 2]. The dynamics of photoemission from free nanoparticles leading to processes occurring in the femto- and atto-second regimes will be briefly mentioned. This requires the use of free electron lasers and ultra-short laser pulses [3, 4].

Nanoscopic matter can also be formed in levitated supersaturated and supercooled microdroplets for investigating nucleation processes in metastable liquids. Structural properties of pre-nucleation clusters are identified by a combination of near-edge spectroscopy and molecular dynamics calculations [4]. In the role of excess charges on the nucleation of liquid microdroplets has been evaluated, since these influence massively the nucleation processes [5].

Finally, topical drug delivery into skin probed by label-free spectromicroscopy is reported. The role of drug formulations and responsive polymeric nanocarriers as efficient drug transport vehicles is evaluated regarding their penetration into deeper skin layers [6, 7]. Selective and high spatial resolution detection of drugs and drug nanocarriers is accomplished by X-ray microscopy and complementary methods, such as atomic force microscopy-based spectroscopic approaches in the infrared regime [8, 9] and stimulated Raman microscopy [10]. Recent results on the penetration of anti-inflammatory drugs are reported, where the drugs are topically applied to human and murine skin samples ex vivo, reaching a spatial resolution below 10 nm.

[1] E. Antonsson, et al., J. Phys. Chem. A 122, 2695 (2018).
[2] C. Raschpichler et al., J. Phys. Chem. C 124, 1664 (2020).
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Lecture 8

High energy/power density lithium-ion batteries through interface engineered CoO@3D-NRGO pseudocapacitive anodes

Venkata Sai Avvaru, Vinodkumar Etacheri

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Although secondary Li-ion batteries are widely used for electrochemical energy storage, their low energy (100-300 Wh kg^{-1}) and power density (250-400 W kg^{-1}) are limiting applications in several areas including long-range electric vehicles [1,2]. In this work, we demonstrated a high energy (400 Wh kg^{-1}) and power density (1 kW kg-1) rechargeable Li-ion full-cell based on extremely pseudocapacitive CoO hybrid anode [3]. These values are 2.8-fold and 2.3-fold higher respectively compared to graphite/$LiCoO_2$ full cells under similar experimental conditions. Three-dimensional anode architecture composed of ultrafine CoO nanoparticles (~10 nm) chemically bonded to nitrogen-doped reduced graphene-oxide (CoO@3D-NRGO). This hybrid anode demonstrated extremely high pseudocapacitance (up to 92%), excellent specific capacity (1429 mAh g^{-1} at 25 mA g^{-1}), rate performance (906 mAh g^{-1} at 5 A g^{-1}), and long-term cycling stability (110% of the initial capacity after 7500 cycles at 5 A g-1). This 3D electrode exhibited outstanding specific capacities and rate performance compared to any of the transition metal-oxide based anodes reported earlier. Long-term cycling stability and coulombic efficiencies are also excellent. Unusual Li-ion storage performances are credited to the synergy between conversion reaction of CoO and pseudocapacitive Li-ion storage at numerous Li_2O/Co/NRGO nanointerfaces resulting from the dispersion of ~3 nm sized Co nanoparticles in Li_2O matrix, and efficient charge separation aided by Co-O-C bonds. Stupendous pseudocapacitance enhanced electrochemical performance of CoO@3D-NRGO hybrid anode makes it a potential candidate for next generation high energy/ power density and ultra-long-life Li-ion batteries. The demonstrated strategy of interfacial engineering can also be extended for other environmental friendly/ inexpensive transition metal oxide (Fe_2O_3, MnO_2 etc.) anodes for high energy/ power density and ultra-long-life Li-ion batteries.

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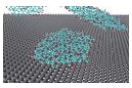


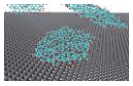
Lecture 9

Humidity responsive Polymer/Gold nanoparticles based hybrid Aerogel for real time Monitoring of Human breath

Israt Ali, Youju Huang, Tao Chen

University of Chinese Academy of Sciences
State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences

Humidity sensor has received considerable attention in recent years because of its significance for air monitoring in agriculture, industries, goods stores and medical detections. Herein, we developed a simple, low cost and scalable fabrication strategy to construct a highly sensitive humidity sensor based on gold nanoparticles (AuNPs) and polymer system, by taking the advantage of conductivity and high surface area of gold aerogel. Such aerogel was fabricated by simple freeze drying method and showed conductivity, highly porous and low density structure. The combined gold nanoparticles (AuNPs) and Poly-N-isopropylacrylamide aerogel shown high sensitivity to water molecules due to the presence of amide group in PNIPAm. Interestingly, this report presents that the facile design of gold aerogel humidity sensor can be used to detect human breath under different health states such as sickness, high breath diseases, lungs problem and respiratory system problems, which is promising in practical flexible wearable devices for human health monitoring. In addition, the promising advantage of gold aerogel allow us in whistle tune recognition application.



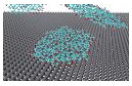
Lecture 10

Engineering of electronic and magnetic properties in all carbon nanostructures

Oliver Gröning

Empa Materials Science and Technology

Graphene provides an ideal platform to create materials with diverse electronic properties by rational control of its nanoscale structure. Quantum confinement effects can be exploited in strictly planar 2D (e.g. porous graphen) or 1D (graphene nanoribbon GNR) graphene structures. However, in order to achieve well defined electronic properties with high electron motilities the nanostructures need to be synthetized with atomic precision.
We will discuss the strategy of using on-surface synthesis to create atomically precise graphene derived nanostructures with non-trivial structures. Based on the flexibility of this approach we will show how specific electronic and even magnetic properties can be engineered and characterized using Scanning Probe Microscopy (SPM) and Scanning Tunneling Spectroscopy (STS).



Lecture 11

Lab-on-a-Chip Systems in Precision Medicine and Personalized Diagnostics

Peter Ertl

TU Wien

Precision medicine or personalized diagnostics uses the information from a patient’s genotype and selected biomarkers to initiate a preventative measure against the development of a disease or select the most appropriate therapy that is particularly suited to a patient. Despite proven benefits of taking personalized medicine approaches, DNA testing and companion biomarker diagnostics have both fall short of their initial promises to increase drug efficiencies in clinical trials, reduce drug failure rates and improve clinical outcomes. To advance precision medicine information of the patient’s own cells are used to identify suitable drug candidates and concentrations in an attempt to predict therapy outcomes. In course of the presentation various organ-on-a-chip systems will be presented using either primary cells or iPSC derived from patients to predict the efficacies of drug candidates.

Lecture 12

Thiolate-protected metal clusters: Chirality and dynamic nature

Thomas Bürgi

University of Geneva

Chirality at the nanoscale has gained considerable interest in recent years. Chiral nanomaterials have properties that are of interest for applications in chiral technology but also in materials science. In this contribution we will focus on a special class of materials: Thiolate-protected metal clusters. These atomically well-defined objects could be used as building blocks for nanotechnology, as catalysts or as sensors. We will discuss the preparation of chiral gold clusters [1], their chiroptical properties and the transfer of chirality within the ligand shell as well as between cluster and ligand [2].

These clusters, although stable, turn out to be very dynamic. The latter is evidenced by the exchange of metal atoms and ligands between clusters as well as between clusters and surfaces. In addition, chiral clusters can undergo racemization. The latter property is usually unwanted but we will show that the interplay between racemization of a cluster and exchange of a chiral ligand can lead to chiral amplification.

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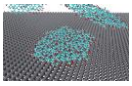


Lecture 13

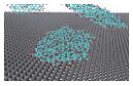
Antibacterial Surface Structures of Cicada Wings and Technical Replication.

Alexander M. Bürger, Richard van Nieuwenhoven, Ille C. Gebeshuber

Technical University - E 134

Recent studies show that the wings of some insects such as cicadas and dragonflies reveal amazing properties. Not only are they super-hydrophobic, comparable to the famous lotus leaf, but also capable of actively killing bacteria. The underlying mechanism is not a chemical bactericide, but tiny nanostructures that mechanically destroy the bacterial cells.

This study will investigate the surface structure of two New Zealandian cicada species (Amphipsalta cingulata and Kikihia scutellaris) with various methods such as AFM. The main focus lies on the investigation of antibacterial structure properties via bacterial tests and on establishing low-cost bioimprinting technique to transfer these structures to artificial surfaces which would open a huge field of manifold applications such as hospital surfaces, medical instruments, smartphone displays and door handles.



Lecture 14

Austrian R&D-Policy in Nantechnology

Alexander Pogany

Federal Ministry for Climate Action, Environment, Energy, Mobility, Innovation and Technology

The Presentation will give an overview about the Austrian R&D-Policy in nanotechnology and Advanced Materials. This includes funding instruments like the R&D-Program "Production of the future" and the M-ERA-Net and initiatives in the area of Nanosafety research like the project NanoTrust and the Nano-EHS-Program.

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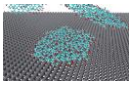


Lecture 15

Investigation of dual-phase TiO2 nanosheet as pseudocapacitive cathodes for Long lasting Mg-Li hybrid batteries.

Mewin Vincent[1,2], Venkatta Sai Avvaru[1,2], Vinodkumar Etacheri[1]

[1] IMDEA materials institute, Madrid, Spain
[2] University of Autonoma, Madrid, Spain

Magnesium batteries attracted great interest as post lithium technology due to its large theoretical volumetric capacity (3833mAh/cm^3), natural abundance (2.7%) low material cost (~$2/Kg) and dendrite free redox reactions. However, the practical Mg-batteries exhibit poor redox activity owing to the slower Mg-ion diffusion kinetics. Mg-Li hybrid batteries are a promising adaptation to fully exploit cost-effectiveness and safety credentials. However, it is a challenging task due to the lack of dual ion compatible high-performance cathode. Herein, we present a long-lasting Mg-Li hybrid battery based on a dual-phase hierarchical TiO2 nanosheet cathode. An optimized dual-phase hierarchical TiO2 nanosheet cathode composed of anatase-bronze polymorphs exhibited excellent electrochemical performance. Nanointerfaces at the polymorphic grain boundaries impart exceptionally higher pseudocapacitive (up to 92%) characteristics. The dual-phase hierarchical cathode demonstrated excellent specific capacities (232 mAh/g at 25 mA/g) and rate performance (120 mAh/g at 1A/g). Further, it showed cycling stability of up to 3000 cycles at 1A/g current density with ~87% capacity retention and ~100% coulombic efficiency. These outcomes are vastly superior to the earlier TiO_2 based Mg-Li hybrid battery cathode investigations. The specific electrode designs imparting good structural robustness is also contributed to the electrochemical characteristics during the charge-discharge process. Exceptional electrochemical characteristics of dual-phase TiO_2 nanosheet cathode is a result of the predominant pseudocapacitive type Mg/Li storage felicitated by the better diffusion of ions through nanointerfaces between anatase and bronze nanocrystallites.

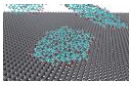
Lecture 16

NanoSolveIT: Nanoinformatics Hazard, EcoTox and Exposure Models

Antreas Afantitis

NovaMechanics Ltd

Technological advances have resulted not only in the development of a multitude of novel and complex nanomaterials (NMs), but also exponential growth of available data. While the unique properties of NMs have led to a large number of commercial applications, a paucity of comprehensive risk and hazard data may lead to adverse effects for humans and the environment. Full exploitation of the available data using in silico tools can assist with NMs assessment and the development of safe-by-design approaches, leading to specific Integrated Approaches to Testing and Assessment (IATA) . The NanoSolveIT project (www.nanosolveit.eu) uses available NM databases and libraries, identifies and fills existing gaps and exploits these data to develop tools that address the needs of regulatory agencies and industry to understand and predict the exposure, hazard and risk from NMs and nano-enabled products, and facilitate computational ‘safe-by-design’ approaches to NMs



Lecture 17

Spider Silk: A nature given advanced material

Aida Naghilou[1], Lena Pöttschacher[2], Flavia Millesi[1], Anda Mann[1], Paul Supper[1], Lorenz Semmler[1], Ellen Backus[2], Christine Radtke[1]

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[2] Department of Physical Chemistry, University of Vienna

Spider silk has been established as one of nature’s most fascinating materials. It has been used in applications such as fishing and wound healing for centuries and in recent years has attracted vivid attention due to its unique strength, toughness, and elasticity [1]. One of the more remarkable applications of the spider silk in medicine, is its use for nerve growth and nerve regeneration [2]. When used as a luminal filling in nerve guidance conduits, spider silk shown peerless success in supporting nerve regeneration [3]. However, the interaction mechanisms between the cells and the silk are still unknown and therefore the reasons behind the medical success of the silk is unclear. This renders a targeted production of synthetic alternatives, such as recombinant silk out of reach.

By comparing different spider silks, material characteristics that promote nerve regeneration can be identified. We performed systematic studies for the silk from spiders Nephila Edulis, and Avicularia avicularia. This combination of fundamental investigations of material properties with the in vitro experiments, delivers a tool for optimum material choice and also a basis for potential material improvement or material synthesis for nerve regeneration applications.

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Lecture 18

QTY code: A simple tool for designs of water-soluble membrane protein, unexpected discovery of truncated receptors that retain biological functions

Shuguang Zhang

Media Lab, Massachusetts Institute of Technology

Structure and function studies of membrane proteins, particularly G protein-coupled receptors (GPCRs) and multipass transmembrane proteins, require detergents. We have devised a simple tool, the QTY code (glutamine, threonine and tyrosine), for designing hydrophobic domains to become water-soluble without detergents. The QTY code designed detergent-free chemokine receptors may be useful in many applications including designing biologics to treat cancer, autoimmune, or infectious diseases. The QTY code allows membrane proteins to be systematically designed through simple, specific amino acids substitutions. The QTY code is robust and straightforward: it is the simplest tool to carry out membrane protein design without sophisticated computer algorithms. Thus, it can be used broadly. The QTY code has implications for designing additional GPCRs and other membrane proteins, or potentially for rendering soluble water-insoluble and aggregated proteins. Furthermore, it has been generally believed that functionalities of GPCRs require full-length sequences. We showed that significantly truncated nfCCR5QTY and nfCXCR4QTY still bind native ligands. Receptor-ligand interactions were discovered from yeast-2-hybrid screening and confirmed by mating selection. Two nfCCR5QTY and two nfCXCR4QTY were expressed in E. coli. Synthesized receptors exhibited alpha-helical structures, and bound respective ligands with reduced affinities. These truncated receptors were reconverted into non-QTY forms and expressed in HEK293T cells. Reconverted receptors localized on cell membranes and functioned as negative regulators for ligand-induced-signaling when co-expressed with full-length receptors. CCR5-SZ190b individually can perform signaling at a reduced level with higher ligand concentration. Our findings provide insight into essential structural components for CCR5 and CXCR4 functionality, while raising the possibility that non-full-length receptors may be resulted from alternative splicing and that pseudo-genes in genomes may be present and functional in living organisms.

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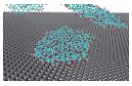

	Monday, January 11, 2021	**Tuesday, January 12, 2021**
9^{00} - 9^{30}	Welcome	Lecture 9 Ali
9^{30} - 10^{00}	Lecture 1 Galteland	Lecture 10 Gröning
10^{00} - 10^{30}	Lecture 2 Baglioni	Lecture 11 Ertl
10^{30} - 11^{00}	Coffee Break	Coffee Break
11^{00} - 11^{30}	Lecture 3 Suzer	Lecture 12 Bürgi
11^{30} - 12^{00}	Lecture 4 Al-Shamery	Lecture 13 Bürger
12^{00} - 13^{00}	Lunch Break	Lunch Break
13^{00} - 13^{30}	Lecture 5 Gebeshuber	Lecture 14 Pogany
13^{30} - 14^{00}	Lecture 6 Parlinska-Wojtan	Lecture 15 Vincent
14^{00} - 14^{30}	Coffee Break	Lecture 16 Afantitis
14^{30} - 15^{00}	Lecture 7 Rühl	Coffee Break
15^{00} - 15^{30}	Lecture 8 Avvaru	Lecture 17 Naghilou
15^{30} - 16^{00}		Lecture 18 Zhang
16^{00} - 16^{30}		Summary