SERS Round Table 2013 in Poltersdorf

October 08-10

Tuesday, 08 October 2013

5:00 pm	**Hiking tour**	
7:00 pm	**Dinner**	
8:00 pm	**Introduction and Evening lecture**	
	Andreas Otto	"Mosel, Poltersdorf and wine"
	Steven Bell	"Working with the Surface in Surface-Enhanced Raman"

Wednesday, 09 October 2013

8:00 am	**Breakfast**	
9:00 am	**Talks and discussions**	
	Janina Kneipp	"SERS for studies of nanoparticle-cell interactions"
	Sumeet Mahajan	"Targeted Nanoprobes for Intracellular SERS"
11:00 am	**Coffee break**	
	Talks and discussions	
	Simion Astilean	"Chitosan-coated triangular silver nanoparticles - a novel class of biocompatible platforms for intracellular SERS sensing and imaging, and plasmonic-mediated hyperthermia"
	Dana Cialla	"SERS as analytical tool"
	Andrea Toma	"Three-Dimensional plasmonic nanostructures for surface enhanced infrared and Raman spectroscopy"
1:00 pm	**Lunch**	
2:00 pm	**Talks and discussions**	
	Santiago Sanchez-Cortes	"Strategies to increase the detection power of plasmonic nanoparticles by SERS and SEF"
	Christoph Haisch	"Considerations on quantitative analysis by SERS"
4:00 pm	**Coffee break**	
	Talks and discussions	
	Pietro G. Gucciardi	"Plasmon enhanced spectroscopy using linear gold nanoantennas with two spectrally distinct resonances: polarization properties and applications to simultaneous SERS and SEIRS molecular detection "
	Annemarie Pucci	"What limits plasmonic enhancement of infrared vibrational signals?"
	Hans-Georg Mack	"Multiscale Approach for Calculating of SERS Spectra (A Brief survey)"
7:00 pm	**Dinner**	

8:00 pm	**Evening lecture** presented by Andreas Otto	
	"Two sources of the SERS background, for rough and smooth samples"	

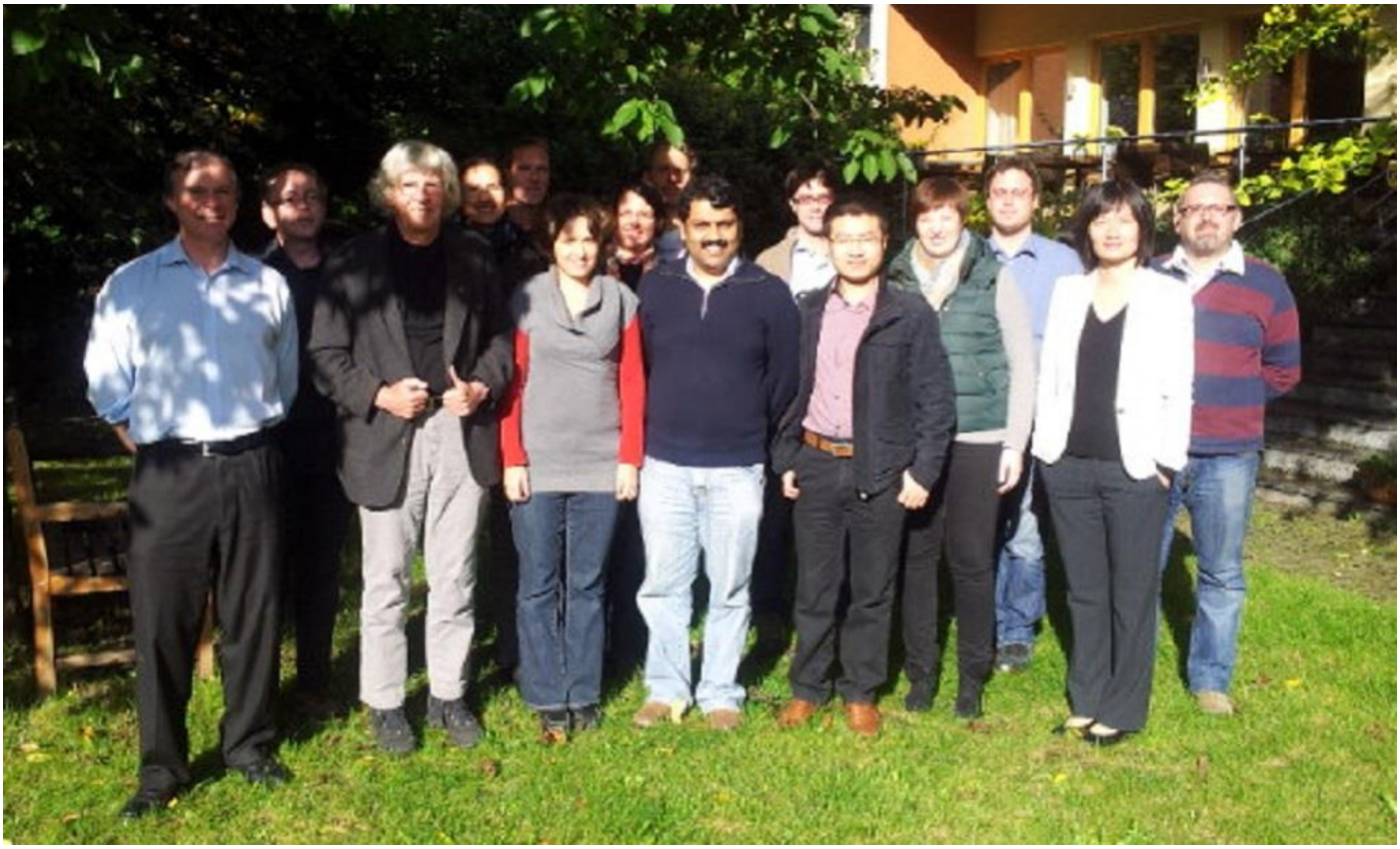
Thursday, 10 October 2013		
8:00 am	**Breakfast**	
9:00 am	**Talks and discussions**	
	Wei Xie	"Rationally designed bifunctional nanoprobes for online monitoring of catalytic reactions by SERS"
	Dai Zhang	"Interaction between organic semiconductor thin film and plasmonic nanostructure"
11:00 am	**Coffee break**	
	Talks and discussions	
	Inez Weidinger	"TiO_2 based electrodes for SERR spectroelectrochemistry "
	Simona Cinta Pinzaru	"SERS in complex biomedia: additive or concurential mechanism? The case of seawater"
	Sebastian Schluecker	"Immuno-SERS microscopy: From the design of SERS labels to tissue-based cancer diagnostics"
	Closing remarks and group photo	
1:00 pm	**Lunch**	

Confirmed participants:

Simion Astilean (Cluj-Napoca)
Steven Bell (Belfast)
Svetlana Brem (Essen)
Dana Cialla (Jena)
Simone Cinta Pinzaru (Cluj-Napoca)
Pietro Giuseppe Gucciardi (Messina)
Christoph Haisch (Munich)
Janina Kneipp (Berlin)
Hans-Georg Mack (Tuebingen)
Sumeet Mahajan (Southampton)
Andreas Otto (Poltersdorf/Duesseldorf)
Annemarie Pucci (Heidelberg)
Santiago Sanchez-Cortes (Madrid)
Sebastian Schluecker (Essen)
Florian Selbach (Essen)
Andrea Toma (Genua)
Inez Weidinger (Berlin)
Wei Xie (Essen)
Dai Zhang (Tuebingen)

Hotel and directions:

For travel information and room reservation please look here:
Hotel Weingut Dehren
Kurfuerstenstrasse 30
56821 Ellenz-Poltersdorf



Abstracts:

Janina Kneipp, "SERS for studies of nanoparticle-cell interactions"

SERS can be utilized for the analysis of cellular samples of plant and animal origin. Specifically, the molecule-SERS substrate interaction can be studied in detail. The talk will cover the interaction of silver nanoparticles with different cellular structures. As will be shown for hemoglobin and red blood cells, the nano-bio-interaction may have serious consequences for biomolecular structure and physiology.

Sumeet Mahajan, "Targeted Nanoprobes for Intracellular SERS"

Nanoparticles functionalized with specific localization signal peptides can be used to target specific organelles inside cells. We use this approach to localize SERS nanoprobes to the nucleus and cytoplasmic organelles. This allows us to monitor biochemical changes which give distinct signatures dependent on the differentiation status of different cell types. I will describe our research on how with generic approach can be applied to a whole range of intracellular investigations and give new fundamental insight.

Simion Astilean, "Chitosan-coated triangular silver nanoparticles - a novel class of biocompatible platforms for intracellular SERS sensing and imaging, and plasmonic-mediated hyperthermia-"

In this work we report a class of biocompatible “optically hot” nanoparticles that are efficient for both plasmonic-induced hyperthermia in NIR and spectroscopic intracellular investigation via SERS and dark-field microscopy. By integrating the advantages of multimodal optical responsivity with targeted hyperthermia, chitosan-coated triangular silver nanoparticles are valuable candidates for applications in nanomedicine.

Dana Cialla, "SERS as analytical tool"

Droplet-based microfluidics in combination with surface enhanced Raman spectroscopy (SERS) and the application of solid SERS substrates are central topics of our research. Within this contribution, the analysis of food additives such as vitamins or food dyes is introduced based on enzymatic generated nanoparticles as SERS platform. A detection scheme for water-insoluble food dyes based on lipophilic sensor layers is discussed. Moreover, monitoring of low-molecular weight substances such as cancer drugs using a microfluidic SERS device and colloidal silver nanoparticles as SERS substrate is introduced.

Andrea Toma, "Three-Dimensional plasmonic nanostructures for surface enhanced infrared and Raman spectroscopy"

The fabrication of complex 3D plasmonic nanostructures integrated in innovative device architectures represents a multidisciplinary key activity at the core of most research efforts in nanoscience and technology. Here we would like to present a novel manufacturing process capable of defining three-dimensional nanostructures/nanocavities made of noble metals of various shapes and spatial arrangements. The process is robust and enables to structure nanomaterials into unconventional geometries whose characteristic length varies from hundreds of nm (visible range) up to few tenths of μm (mid-infrared). The proposed architectures can offer new and unconventional properties such as the realization of high electric field confinement and enhancement, finely structured extinction profiles, broad-band optical absorption, strong radial scattering and well defined radiation pattern. Moreover, we investigated and exploited the unique properties of these nanoplasmonic structures to improve the vibrational signal enhancement in plasmon-assisted Raman and infrared spectroscopy.

S. Sanchez-Cortes, "Strategies to increase the detection power of plasmonic nanoparticles by SERS and SEF"

The strong intensification of the electromagnetic field in the presence of nanoparticles (NPs) with plasmonic properties results in a substantial enhancement of the effective cross section in the case of certain optical spectroscopy applied to the analysis of molecular systems. This is the case of mainly Raman scattering, in SERS (Surface-Enhanced Raman Scattering) and the fluorescence emission, which is known as SEF spectroscopy (Surface-Enhanced Fluorescence) when it is carried out in the presence of these nanoparticles. The above techniques have interesting applications in many fields like molecular detection and the study of interfacial phenomena.
In the present work we propose strategies to further increase the cross section of the above techniques. The nanofabrication of anisotropic NPs and the molecular linking of nanoparticles are two interesting options to take into account in this sense.
Nanofabrication of anisotropic NPs, mainly triangular nanoprisms and nanostars, is currently an interesting field of research in the frame of SERS and SEF techniques. On these nanosystems, strong enhancement factors can be achieved without the need of a previous activation. Recently, we have developed in our group nanofabrication protocols to obtain nanostars of Ag and bimetallic Ag@Au ones, with a high SERS performance. Another strategy for increasing the performance of these nanoparticles is their assembly by means of bifunctional molecules leading to the formation of interparticle spaces or gaps, which produces a high intensification of the field, also called hot spots. These systems can be induced by functionalization of NPs with aliphatic bifunctional molecules (diamines, dithiols and dicarboxylates) or aromatic linkers (viologens, disulfides and diisocyanides). These molecules have two different roles: a) NPs linking to create hot spots; and b) the molecular hosting inside the interparticle gaps aimed to detect compounds of interest and eventually inducing photocatalysis processes on the molecules allocated inside such cavities.

Christoph Haisch, "Considerations on quantitative analysis by SERS"

In any textbook on analytical chemistry, the concept of quantitative analysis and a Limit of Detection (LOD) is discussed. In practice, this parameter is often hard to determine. A major advantage of SERS is its high information content, encoded into the spectrum. However, this raises the question of how to calculate an LOD when a selective analysis requires for full-spectra evaluation. Possible solutions are discussed on two examples.

Pietro G. Gucciardi, "Plasmon enhanced spectroscopy using linear gold nanoantennas with two spectrally distinct resonances: polarization properties and applications to simultaneous SERS and SEIRS molecular detection"

Annemarie Pucci, "What limits plasmonic enhancement of infrared vibrational signals?"

Many IR studies show enhanced vibrational signal from various more or less sophisticated plasmonic structures but all arrive at enhancement factors below 1 000 000. Three issues will be discussed: First, crystallinity of the plasmonic particles may be a limiting factor. Second, damping and disorder in the vibrational system should be important. Third, there seems to be an optimum distance from the metal surface for maximum enhancement.

Hans-Georg Mack, "Combined Quantum Mechanics and Classical Electrodynamics Multiscale Approach for Calculating of SERS Spectra (A Brief survey)"

The challenge to build a theory for calculating SERS optical response that inclu-des both quantum mechanics (QM) and electrodynamics (ED) lies with the fact, that the length scales needed for the two calculations differ in order of magnitude. Purely chemical models of SERS based on QM methods are

generally limited to ~1 nm in size, including the metal particle/cluster, while electromagnetic field evaluations are usually based on grids or finite elements, that have 1 nm dimensions at the minimum. For this reason, theoretical treatments of SERS often take one of two paths: One ap-proach neglects the CHEM enhancement and focuses on the predominant EM enhan-cement, while other studies only determine the CHEM enhancement using a small ato-mic cluster model of the nanoparticle.
Much of current research in this field focuses on novel multiscale methods for analysis and understanding SERS mechanisms by combination of quantum mechanics (RT-TDDFT, LR-TDDFT) and classical electrodynamics (f.i. FDTD). The RT-TDDFT/ FDTD model will be briefly discussed here.

Andreas Otto, "Two sources of the SERS background, for rough and smooth samples"

The holistic model of SERS connects, without antagonism, the additional electronic enhancement at SERS active sites with the electromagnetic enhancement. In well produced nanostructures in air there is only long range EM enhancement and a small concentration of SERS active sites, which are quenched by oxygen. This model predicts a continuous background induced by molecular adsorption on smooth noble metal surfaces, which is enhanced by the plasmonic near field like the intensities of the Raman bands. We present experimental evidence for this interpretation. A very different background is observed at rough surfaces without adsorbates and without any change of intensity by adsorption. This background disappears when the roughness is annealed.

Wei Xie, "Rationally designed bifunctional nanoprobes for online monitoring of catalytic reactions by SERS"

SERS is a surface-selective technique with high sensitivity and chemical specificity which fulfills the requirements for in situ monitoring of molecular transformations in heterogeneous catalysis. However, catalytically active materials such as Pt, Pd, and small Au NPs do not provide sufficient plasmonic activity for the required SERS enhancement.
On the other hand, conventional SERS substrates such as large Au or Ag NPs are not catalytically active. In our lab, the catalysts NPs are self-assembled on a large plasmonically active core to form a plasmonic superstructure; in this case the chemical species on the catalyst surface experiences a sufficient SERS enhancement due to the plasmonic coupling between the small satellites and the large core.

Dai Zhang, "Interaction between organic semiconductor thin film and plasmonic nanostructure"

Intense attentions have been given to the nanoantenna systems, due to their fascinating plasmonic properties, light confinement abilities, and wide applications in sensor, energy conversion (solar and catalysis), and high resolution optical spectroscopy.
In my talk, I will discuss about the linear- and non-linear optical properties of metallic nanoantenna. Photoluminescence emission, two photon photoluminescence and second harmonic generation of nanoparticle dimmers will be shown. Furthermore, I will demonstrate our latest research work about probing local structural order of semiconductor thin films and their interactions with plasmonic nanostructures using polarized Raman spectroscopy.

Inez Weidinger, "TiO_2 based electrodes for SERR spectroelectrochemistry"

In my talk I will show the potential of nanostructured TiO_2 electrodes as a biocompatible support for SERR spectroelectrochemistry of surface bound proteins. While the surface enhancement of the TiO_2 electrodes clearly stays below the enhancement generated by plasmonic noble metals, a clear dependence of the SERR signal on surface morphology can be seen. Furthermore I will show how SERR enhancement and conductivity of these electrodes can be tuned by attaching TiO_2 films to nanostructured silver and gold supports.

Simona Cinta Pinzaru, "SERS in complex biomedia: additive or concurential mechanism? The case of seawater"

The possibility to SERS detect a sume of both organic and inorganic species in a mixture, including aggregation agents is discussed. One of the most complex biosystem behavior, seawater is analyzed, by experimentally substracting the salts and microorganisms (phytopankton) contribution from overall signal, aiming to provide a correct interpretation and assignment of the complex SERS spectra.

Sebastian Schluecker, "Immuno-SERS microscopy: From the design of SERS labels to tissue-based cancer diagnostics"

Surface-enhanced Raman scattering microscopy (µSERS) employs target-specific colloidal SERS probes in combination with Raman microspectroscopy. For example, SERS-labeled antibodies allow the selective and sensitive localization of the corresponding antigen in tissue specimens. The physical and chemical properties of the colloidal SERS probes are crucial for the success of SERS microscopic experiments. Stability and robustness, sensitivity as well as steric accessibility for bioconjugation are few very important aspects. One option for increasing colloidal stability of SERS nanoparticles is the use of hydrophilic ethylene glykole spacers covalently attached to the Raman reporter molecules. A second approach is the encapsulation by silica. Both types of SERS probes were optimized for red laser excitation in order to improve image contrast by minimizing disturbing autofluorescence of biological specimens. Two different routes to the glass encapsulation of a complete monolayer of Raman reporters on the metal surface will be described. Small clusters (dimers, trimers) of gold nanocrystals even exhibit single-particle sensitivity and enable rapid mapping experiments with only 30 msec acquisition time per pixel. Imaging results on tissue sections from the benign prostate demonstrate the selective abundance presence of the tumor suppressor p63, a p53 homologue, in the basal cells of the epithelium. Future directions of this innovative Raman/SERS microspectrosopic technique for tissue-based tumor diagnostics will be discussed.