

PLASMOCAT

Nanoplasmonics for Catalysis

Strasbourg, November 23-24, 2026

Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS)

“Salle 74”, ground floor

GENERAL INFORMATION

Objectives

As part of the "**Nanoplasmonics for Catalysis**" project, funded by the CNRS Mission for Transverse and Interdisciplinary Initiatives, we are organizing a two-day workshop on this topic. This workshop will bring together a variety of experts—physicists and chemists, theoreticians and experimentalists—in the field of photoactivable and photocatalytic nanomaterials.
This workshop aims to be a forum for reflection and discussion on the state of the art in the description of plasmon-induced photophysical and photochemical phenomena. It will focus in particular on modelling and measuring (i) light-matter interactions (ii) photoinduced charge carrier dynamics, and (iii) photoinduced chemical reactivity of the surface.

Organisers

Valérie Caps (ICPEES) and Giovanni Manfredi (IPCMS)

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Venue

Institut de Physique et Chimie des Matériaux de Strasbourg (Salle 74, ground floor), CNRS Cronenbourg Campus, Strasbourg.

INVITED SPEAKERS

Miguel Comesana-Hermo, ITODYS (Interfaces Traitements Organisation et Dynamique des Systèmes), Paris

Stefano Corni, Department of Chemical Science, University of Padova

Petra Hellwig, Chimie de la Matière Complexe, Université de Strasbourg

Paul-Antoine Hervieux, Institut de Physique et Chimie des Matériaux, Université de Strasbourg

Jun Huang, Institute of Energy Technologies, Forschungszentrum Jülich

Mathieu Kociak, LPS (Laboratoire de Physique des Solides), Paris

Stefan Kümmel, Faculty of Mathematics, Physics and Computer Sciences, University of Bayreuth

Olivier Pluchery, INSP (Institut des Nanosciences de Paris), Sorbonne Université

Rajarshi Sinha Roy, Institut Lumière Matière, Université Lyon 1

Hans-Christian Weissker, CiNAM (Centre Interdisciplinaire de Nanoscience de Marseille)

PROGRAM

	Monday 23/11	Tuesday 24/11
Venue	*IPCMS - salle 74*	*IPCMS - salle 74*
9:00		**Olivier Pluchery**
9:40		**Mathieu Kociak**
10:20	*Welcome*	**Rajarshi Sinha Roy**
11:00	**Miguel Comesana-Hermo**	*Discussion*
12:00–14:00	*Lunch*	*Lunch*
14:00	**Stefan Kümmel**	**Petra Hellwig**
14:40	**Hans-Christian Weissker**	**Jun Huang**
15:20	*Discussion and coffee break*	*Discussion and coffee break*
16:00	**Paul-Antoine Hervieux**	End
16:40	**Stefano Corni**	
17:20	*Discussion*	
18:00		
19:00	*Dinner at Maison Kammerzell*	

ABSTRACTS

Miguel COMESANA-HERMO

***Title**: Limitations and opportunities of plasmonic catalysis*

Abstract: Plasmonic catalysis has emerged as a rapidly evolving field of research that harnesses the unique optoelectronic properties of plasmonic nanomaterials to activate and modulate chemical reactivity. In particular, the generation of highly energetic charge carriers and the confinement of electromagnetic fields at the surface of these objects offer unprecedented control over the efficiency and selectivity of diverse chemical transformations. Despite this remarkable potential, plasmonic catalysis faces several intrinsic limitations that continue to hinder its translation into practical applications. In this seminar we will examine the key challenges of plasmonic catalysis, discuss strategies to mitigate them, and outline emerging directions where this reactivity hold significant promise.

Stefano CORNI

***Title:** Changing molecular reactivity with plasmons: insights from multiscale modeling*

Abstract: Plasmonic nanostructures are known to affect the properties of nearby molecules through various mechanisms. They modify plasmon-resonant external electromagnetic fields by enhancing their local intensity close to the nanostructure, in particular inside gaps (hot-spots). Such effect also applies to fields emitted by the molecule, amplifying molecule-plasmon energy transfer up to the point of reaching the molecule-plasmon strong coupling regime. Finally, photoexcitation of plasmons may result in charge carrier transfer to the molecule by direct or indirect processes, leading to reactive molecular species. The different length and time scales involved, as well as the complexity of the underlying mechanisms, call for multiscale descriptions of these systems. Through the years we have developed PCM-NP, a multiscale model based on an atomistic quantum chemical treatment of molecules coupled to a simplified continuum representation of the plasmonic nanostructures. In this talk such approach will be introduced and some relevant applications discussed.

Petra HELLWIG

Title: *Nanostructured SERS and SEIRAS Platforms for Advanced Monitoring of Membrane Proteins*

Abstract: Understanding how membrane proteins function at the molecular level remains a major challenge, largely due to their low abundance, structural complexity, and the difficulty of probing them in physiologically relevant environments. Surface-enhanced infrared absorption spectroscopy (SEIRAS) offers a powerful solution, enabling sensitive investigation of proteins at very low concentrations. However, its performance critically depends on the design of the underlying nanostructured substrate.

To address this challenge, we systematically explore and compare different nanostructured platforms—electrolessly deposited gold nanoparticles[1], graphene nanodots[2], and lithographically defined gold slit nanoantenna arrays [3]—as tailored interfaces for enhanced vibrational spectroscopy of membrane proteins. For gold-based substrates, nanoscale morphology is a decisive parameter: optimal electroless deposition yields isolated nanostructures that maximize signal enhancement, while minor deviations drastically reduce performance. In addition, protein immobilization strategies, such as electrostatic adsorption or Ni–NTA/His-tag coordination, reshape the nanoparticle network into three-dimensional architectures that further enhance signal amplification. Graphene nanodots provide a chemically versatile and stable platform, supporting both SEIRAS and SERS measurements. They enable reliable immobilization of membrane proteins such as cytochrome bd-I oxidase, preserving structural integrity while achieving reproducible signal enhancement and detection limits down to the nanomolar range over several days.

To achieve precise control over plasmonic properties, we further develop gold slit nanoantenna arrays with tunable geometries. By adjusting the slit dimensions, the plasmonic resonance can be positioned across the mid-infrared fingerprint region, resulting in geometry-dependent enhancement in both SEIRAS and SERS without compromising protein structure.

We demonstrated the functional relevance of these optimized platforms by probing, for example the mechanism of lactose permease (LacY). Using SEIRAS, we identified Glu325 as the key residue responsible for the unusually high apparent pKa (~10.5) required for substrate binding, and showed that Arg302 plays a crucial role in its deprotonation, providing direct insight into the coupling between protonation and transport activity.[4]

Together, these results demonstrate that the rational design of nanostructured interfaces enables sensitive, reproducible, and mechanistically informative studies of membrane proteins, opening new perspectives for biosensing and bioenergetics research.

[1] A. F. S. Seiça, M. H. Iqbal, A. Carvalho, J. Y. Choe, F. Boulmedais, P. Hellwig, Study of Membrane Protein Monolayers Using Surface Enhanced Infrared Absorption Spectroscopy (SEIRAS): Critical Dependence of Nanostructured Gold Surface Morphology, ACS Sensors, 2021, 6(8), 2875–2882.

[2] F. Omeis, A. F. Santos Seiça, R. Bernard, N. Javahiraly, H. Majjad, D. Moss, P. Hellwig, Following the Chemical Immobilization of Membrane Proteins on Plasmonic Nanoantennas Using Infrared Spectroscopy, ACS Sensors, 2020, 5(7), 2191–2197; A Murillo Bello, P Hellwig, Length-Tunable Gold Slit Nanoantennas for Surface-Enhanced Vibrational Detection of Cytochrome *bd*-I Oxidase, ACS Applied Nano Materials 9 (24), 11257-11268.

[3] A. Murillo- Bello, A. G. Ricciardulli, A. R. Umar, T. Gerasimova, T. Friedrich, N. Javahiraly, P. Samorì, P. Hellwig, Graphene Nanodots as Substrates for SEIRAS and SERS Studies on Membrane Proteins, Langmuir, 2025, 41, 25, 16468–16476.

[4] N. Grytsyk, A. F. Santos Seiça, J. Sugihara, H. R. Kaback, P. Hellwig, Arg302 Governs the pKa of Glu325 in LacY, Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4934–4939.

Paul-Antoine HERVIEUX

***Title**: Ultrafast control of orbital magnetism in metallic nanoparticles via quantum and semi-classical models*

Abstract: The transfer of angular momentum from helicity-controlled laser fields to non-magnetic electronic systems can induce magnetisation via the inverse Faraday effect. This phenomenon has been investigated in metallic nanoparticles [1,2] and clusters [3] using a semi-classical model (QHD) and a full quantum approach within a many-body framework. Real-time time-dependent density functional theory (TDDFT) was employed, with the nanoparticles modelled using either a spherical jellium approximation on a real-space grid or a realistic atomic structure. Circularly polarised light induces orbital magnetism, peaking at surface plasmon resonance, which confirms its plasmonic origin. The dominant magnetic contribution arises from surface currents; however, quantum-induced bulk effects, such as Friedel oscillations, also persist.

[1] J. Hurst, P. M. Oppeneer, G. Manfredi and P. -A. Hervieux, Phys. Rev. B **98**, 134439 (2018).

[2] R. Sinha-Roy, J. Hurst, G. Manfredi and P. -A. Hervieux, ACS Photonics **7**, 2429 (2020).

[3] L. Deru, Y. Yang, G. Manfredi, P. -A. Hervieux, and R. Sinha-Roy, Nanophotonics **13**, 4291 (2024).

Jun HUANG

***Title**: Localized Surface Plasmon Resonance at Electrochemical Interfaces: A Semiclassical Theory*

Abstract: Electrochemical plasmonics enables in situ optical probing and modulation of electrochemical interfaces. Experiments have shown that the localized surface plasmon resonance (LSPR) at the interface between a metal nanoparticle and an electrolyte solution is sensitive to electrode potential, nanoparticle morphology, electrolyte composition and chemisorption. Theoretical modeling is instrumental to mechanistic understanding of these experimental observations. It has, however, remained challenging to model the LSPR under experimentally relevant conditions. Here, we tackle this challenge by employing an approach based on nonequilibrium density-potential functional theory. The approach is first compared with experimental results for the effects of nanoparticle size and dielectric environment on the LSPR under electroneutral conditions, showing qualitative agreement in the trend, and is then compared with time-dependent density functional theory calculations. Beyond electroneutral conditions, the approach is used to analyze the electrode potential effects on the LSPR. A blueshift at more positive electrode potentials is obtained and is attributed to a steeper gradient of electron density at the interface. In contrast to conventional models that neglect electron spillover, this blueshift indicates that the electron density gradient dominates over the number of electrons in influencing the LSPR. The connection with experimental observations is discussed. Overall, this theoretical approach contributes to establishing a quantitative connection between electrical double layer structure and plasmonic resonance.

Mathieu **KOCIAK**

Title: *How can electron microscopy contribute to the study of nanoplasmonics for catalysis?*

Abstract: Electron microscopy is a key tool for characterizing catalytic particles, providing access to their morphology, structure, chemical composition, and oxidation states, down to atomic resolution. Environmental electron microscopy allows us to track how these properties evolve under conditions that more closely resemble those encountered during catalysis. The growing availability of light illumination within electron microscopes also opens up opportunities for in situ photocatalysis experiments. Meanwhile, electron energy-loss spectroscopy (EELS) and cathodoluminescence offer powerful ways to probe the optical properties of plasmons at spatial scales inaccessible to other techniques. I will begin with a brief overview of electron microscopy applications in catalysis and photocatalysis—a subject in which I may well be no more of an expert than many in the audience. Our group's expertise lies in plasmonics, optical spectroscopies, and laser illumination within the electron microscope. I will present recent developments in these areas and explore, together with the audience, how these methods could help advance the study of nanoplasmonics for catalysis.

Stefan **KUMMEL**

Title*: Insight into Electronic Properties of Light-Converting Systems from Density Functional Theory*

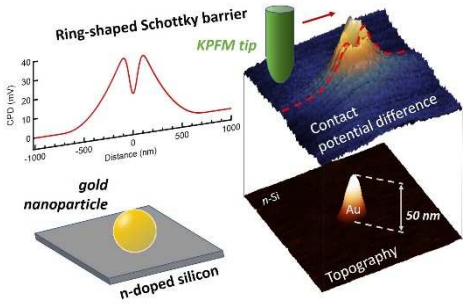
Abstract: Photosynthetic bacteria can convert light with an amazingly high quantum efficiency. Molecular complexes anchored to semiconductor surfaces can improve the efficiency of photoelectrochemical water splitting. This talk will discuss how (time dependent) density functional theory (DFT) can offer insight into the underlying electronic processes. It allows, e.g., to reveal in real-time and real-space the electronic dynamics after an excitation. The talk will furthermore discuss that the accuracy of DFT calculations is decisively determined by the chosen exchange-correlation approximation, and will discuss recent developments that can benefit calculations for energy-converting systems.

Olivier PLUCHERY

***Title**: Plasmonic Excitation and the Local Field at Individual Gold Nanoparticles: Understanding Hot Electron Injection*

Abstract: Plasmonic nanostructures are actively investigated for their optical properties and for a wide range of applications in nanophotonics, biosensing, photocatalysis, hot carrier physics and advanced cancer therapies [1]. The localized surface plasmon resonance (LSPR) can be excited in gold nanoparticles or in more complex nanostructures and gives rise to a wide range of unique optical properties. In particular, there is a strong focus to understand how plasmonic nanostructures enhance the generation of hot electrons and trigger chemical reactivity or enable photocatalytic reaction. It is often critical to be able to localize individual plasmonic nanoparticles and measure their plasmonic spectrum, which is known as hyperspectral microscopy.

In this presentation we explain how we achieved hyperspectral microscopy with an optical microscope equipped with a dark field objective and coupled to an optical spectrometer [2]. Images of spherical gold nanoparticles (diameters 90, 70, 50 and 25 nm) grafted onto a semiconductor, were recorded, along with their scattering spectra. Then, we will show that this architecture behaves like a **nano-size Schottky junction**. The electrostatic properties of this junction were studied with Kelvin Probe Force Microscopy (KPFM) and the local space-charge region was unraveled (see Fig) [3, 4]. These results shed a new light on the mechanisms of hot carried injection.



[1] Pluchery, O.; Bryche, J.-F., *An Introduction to plasmonics*. World Scientific (2023) https://www.worldscientific.com/doi/abs/10.1142/q0395

[2] Abadie, C.; Liu, M.; Prado, Y.; Pluchery, O., Hyperspectral dark-field optical microscopy correlated to atomic force microscopy for the analysis of single plasmonic nanoparticles: tutorial. *J. Opt. Soc. Am. B* **2024,** *41* (8), 1678-1691. https://doi.org/10.1364/JOSAB.523547

[3] Lechaptois, L.; Prado, Y.; Pluchery, O., KPFM visualisation of the Schottky barrier at the interface between gold nanoparticles and silicon. *Nanoscale* **2023,** *15* (16), 7510-7516. http://dx.doi.org/10.1039/D3NR00178D

[4] Zhang, Y.; Pluchery, O.; Caillard, L.; Lamic-Humblot, A.-F.; Casale, S.; Chabal, Y. J.; Salmeron, M., Sensing the Charge State of Single Gold Nanoparticles via Work Function Measurements. *Nano Letters* **2015,** *15* (1), 51-55. https://doi.org/10.1021/nl503782s

Rajarshi SINHA ROY

Title: *Light-Driven Orbital Magnetism in Plasmonic Metasurfaces Based on Sub-Nanometer Building Blocks*

Abstract: Recent advances in spin-orbitronics have highlighted the importance of nonequilibrium processes associated with electronic orbital degrees of freedom. In parallel, experiments [1,2] on metallic nanoparticles have shown that light-driven orbital currents can produce transient magnetization on ultrafast timescales, particularly at plasmonic resonance energies. Motivated by these developments, we investigate plasmonic metasurfaces as a potential platform for generating and controlling light-induced orbital magnetism via the inverse Faraday effect. Employing real-time ab-initio simulations and treating metallic clusters as the fundamental building blocks, we demonstrate that irradiation with an ultrashort laser pulse can generate a pronounced and stable magnetic moment. By systematically varying the cluster dimensions and examining the corresponding near-field characteristics, we identify key structural and electromagnetic parameters that govern the efficiency of orbital magnetization generation. These findings provide design guidelines for engineering plasmonic metasurfaces and suggest new opportunities for constructing functional superlattices from metallic clusters.

[1] Cheng et al., Light-induced magnetism in plasmonic gold nanoparticles, Nature Photonics **14**, 365 (2020).

[2] Parchenko et al., Plasmon-enhanced optical control of magnetism at the nanoscale via the inverse faraday effect, Advanced Photonics Research **6**, 2400083 (2024).

Hans-Christian WEISSKER

Title*: Optical Properties of Gold Clusters Following Surface-Modification by Hydrogen Exposure*

Abstract: The adsorption of hydrogen on small nanoparticles has garnered attention due to its potential applications in catalysis, energy storage, and hydrogen detection. The importance of the surface modifications and of resulting structural transformations under hydrogen exposure have been demonstrated experimentally and studied theoretically [1]. The consequences for the catalytic activity of gold nanoparticles are far-reaching, potentially explaining its size-dependence.

In the present work [2], we study the consequences of the surface modifications following hydrogen exposure on the optical properties. To calculate the optical response, we employ real-time TDDFT+*U* calculations which correct the poor description of the electronic d band of many previous calculations. This has been shown to lead to excellent results for silver clusters of all sizes [3] and also to improve the spectra of plasmonic gold nanoparticles [4].

We discuss, in particular, the distinction of chemical and structural effects of the surface modification. Gold nanoparticles are a well-known efficient plasmonic system when clean and pure. In our present work, we show that the gold nanoparticles lose their strong surface-plasmon resonance upon hydrogen exposure. This effect might possibly be exploited for the realization of gold-cluster-based hydrogen detectors. Furthermore, we identify surface-confined super-atom states in addition to the usual volume super-atom states. The change of the optical properties is, in particular, linked to the loss of super-atom character of the states above the gold d band [4]. The work is expected to lead to a better understanding of the optical properties of noble-metal nanoparticles with chemical surface modifications.

[1] Nassereddine *et al.,* Revealing Size Dependent Structural Transitions in Supported Gold Nanoparticles in Hydrogen at Atmospheric Pressure, *Small* **17,** 2104571 (2021).

[2] Hydrogen-Induced Suppression of the Optical Plasmonic Response in Ultra-Small Gold Nanoparticles, Mohit Chaudhary, Loréna Chabeaud, Ranjan Bassi, Hazar Guesmi, Hans-Christian Weissker, *Phys. Chem. Chem. Phys.* (2026), https://doi.org/10.1039/D6CP00557H

[3] Chaudhary & Weissker, Optical spectra of silver clusters and nanoparticles from 4 to 923 atoms from the TDDFT+*U* method, *Nat. Commun.* **15,** 9225 (2024).

[4] Optical spectra of plasmonic Au clusters and nanoparticles obtained using the TDDFT+*U* method Mohit Chaudhary, Jean Lermé, Hans-Christian Weissker, *Nanoscale* **18,** 5389–5399 (2026).