OSI-13 Scientific Program

Centro de Investigaciones en Óptica
León, Guanajuato, México
June 3-7, 2019

Monday 3

10:00-11:00 **Kenan Gundogdu**: NC State University, USA. **Invited**
Optically Created and Sustained Electron Hole Liquid in Monolayer MoS_2

Many-body interactions in photoexcited semiconductors leads to strongly-interacting electronic states. At the high excitation density limit these interactions leads to formation of fully ionized electron-hole plasma (EHP) and electron-hole -liquid (EHL) phases. EHL is an exotic phase with unique electronic properties, such as metallic conductivity and metastable high photoexcitation density, which can be the basis for future transformative applications. However, the cryogenic condition required for its formation has limited the study of these phases to a purely academic pursuit in a restricted parameter space. This paradigm can potentially change with the recent experimental observation of these phases in atomically thin MoS2 and MoTe2 at room temperature. A fundamental understanding of EHP and EHL dynamics is critical for developing novel applications on this versatile layered platform. In this talk I will present the formation and dissipation of EHL in monolayer MoS2. Unlike in bulk semiconductors, the results presented here reveal that electro-mechanical material changes in monolayer MoS2 during photoexcitation play a significant role in EHL formation. Within the free-standing geometry, photoexcitation is accompanied by an unconstrained thermal expansion, resulting in a direct-to-indirect gap electronic transition at a critical lattice spacing and fluence. This dramatic altering of the material's energetic landscape extends carrier lifetimes by 2 orders of magnitude and allows the density required for EHP formation. The result is a stable dense plasma state that's sustained with modest optical photoexcitation. Our findings pave the way for novel applications based on collective electronic states in 2D semiconductors.

Nano Lett. 19 (2019) 1104

Monday 3

11:00-11:40 **Lucila Juarez**: CIO, México.
Mie scattering in Metamaterials

Small high-refraction-index dielectric inclusions display strong electric and magnetic multipole Mie resonances in the optical region, which could be potentially used as resonators for the fabrication of low loss negative refraction metamaterials. The resonant modes strongly depend on the composition, size and geometry of the particles, allowing for a wide range of possibilities for the design of optical metamaterials. However, the description of Mie scattering lies beyond the long wavelength limit often used to study metamaterials. We present a general numerical approach for the calculation of the effective dielectric function of metamaterials of arbitraty geometry which takes into account retardation and non local effects, allowing the study of metamaterials based on Mie resonances.

Monday 3

12:10-12:50 **Raksha Singla**: ICF-UNAM, México.
SHG from nanoparticles of noncentrosymmetric geometry

The nonlinear polarization resulting in generation of second harmonic (SH) radiation from centrosymmetrical (CS) media mostly takes place at the surface where the inversion symmetry is lost. This local disruption of symmetry disappears globally for a symmetrical particle, suppressing its total SH polarization. In this work, we explore SHG from particles of CS materials with non-CS geometry. We choose an isolated cylindrical particle with a deformed circular cross-section in the presence of an ambient field with a long wavelength. Assuming a small deformation parameter, a perturbative scheme is employed to analytically solve the linear and quadratic field equations, employing the dipolium model to calculate the SH bulk and surface polarization. We report the SH dipolar and quadrupolar hyperpolarizability tensors, their spectra, the radiation patterns, and the conversion efficiency.

Phys. Rev. B 53 (1996) 4999
Phys. Rev. B 99 (2019) 125418

Monday 3

12:50-13:50 **Mahfujur Rahaman**: Chemnitz University of Technology, Germany. **Invited**

Tip-Enhanced Raman Scattering (TERS) of MoS2/Plasmonic Heterostructures: Understanding the TERS Sensitivity and Local Heterogeneities at the Interface

Two dimensional (2D) semiconductors are one of the most extensively studied materials in recent times. This class of materials have astonishing chemical, optical, electronic, and mechanical properties which are different from their bulk counterparts. Due to strong confinement in the out-of-plane directions, local heterogeneities such as edges, grain boundaries, strain, defects, and doping strongly affect the physical properties of these materials. However, investigating such local heterogeneities using conventional optical spectroscopy is hindered due to the diffraction limit of light. Thanks to the improved spatial resolution (down to sub-nanometer), tip-enhanced Raman spectroscopy (TERS) also attracted a lot of interest recently. Since the first reports in the early 2000s, there have been several experimental configurations that have demonstrated high TERS sensitivity in terms of enhancement and spatial resolution. The combination of a plasmonic substrate and a metallic tip is one suitable approach to achieve even higher TERS sensitivity in so called gap-mode TERS. In this contribution, we present our recent works on TERS of MoS2/plasmonic heterostructures to address the approach. The contribution is divided into two parts. In the first part, we discuss the physics of TERS sensitivity on and around the Au nanodisks covered by monolayer MoS2 probed by a metallic tip. Au nanodisks were prepared by electron beam writing and then monolayer MoS2 was transferred onto the plasmonic substrate by a deterministic transfer method. TERS experiments were conducted using 785 nm (1.58 eV) excitation (i.e. much below the band gap of 1L-MoS2; 1.9 eV) with a side illumination/collection geometry. We achieved an unprecedented enhancement of 5 x 108 with a spatial resolution of around 2 nm. To understand the experimental results, finite element method simulation using COMSOL is introduced. Our simulations reproduced the TERS images very well and explains the plasmonic process involved in the experimental system. In the second part, a new approach for measuring the phonon spectra of nanomaterials using TERS in combination with plasmonic substrate is discussed. This allows gigantic enhancement and very good spatial resolution which makes it possible to investigate the influence of local heterogeneities at the 2D/plasmonic interface at the nanoscale. Due to the curvature of the MoS2 film following the morphology of the Au nanodisks during deposition, it is subjected to a strain of about 0.9 %. Moreover, due to strong plasmonic hot electron doping we observed a transition from the semiconducting 1H to the metallic 1T phase in 1L-MoS2 at the hot spots with a maximum temperature rise of 110 ^oC at those hot spots. Thanks to the remarkable TERS spatial resolution in our approach, we were able to locate the site dependent local properties of MoS2 originating from temperature rise, strain, and plasmonic hot electron doping.

Nano Lett. 17 (2017) 6027
Nanoscale 10 (2018) 2755
Faraday Discuss. 10.1039/C8FD00142A

15:30-16:30 **Dmytro Solonenko**: Chemnitz University of Technology, Germany. **Invited**
Raman spectroscopy of functionalized 2D and quasi-1D Si nanostructures grown on Ag surfaces

Recent advancements in the field of 2D materials suggest the opening of new era in nanotechnology, where tuning of physical properties of a crystal can be realized with high precision and over a broad range. Such sensitivity of these materials is dictated by the close relation between their atomic structure and their electronic properties. Therefore, an accurate way to track the structural changes during their functionalization has to be employed in order to deeply understand this dependence. Raman spectroscopy is an well-established method to study nanomaterials in various dimensionalities. In this work, in situ Raman spectroscopy was used to investigate the possibilities of functionalization of 2D Si structure, silicene, and quasi-1D Si structure, Si nanoribbons, which can be grown on Ag(111) and Ag(110) substrates, respectively. Certainly, the vibrational signatures of these structures are different to ones of the bulk Si-related species, hence their rationalization preceded the modification. In order to probe the chemical activity as well as the structural disposition to host foreign atoms, atomic hydrogen and oxygen were chosen as adsorbants. The results show drastic differences in the response of Si allotropes to the adsorbed atomic species, which will be discussed in the talk. The exploration of the structures with Si atoms in the higher bond orders broadens our understanding as well as their applications in the modern microtechnology.

16:30-17:10 **Bruno Wacogne**: FEMTO -ST Institute, France.
Calibration free optical pH sensing using physico-chemical modeling of fluorescein grafted silica fibers

Dual emission wavelengths fluorescent indicators like SNARF allow measuring pH by calculating the ratio of the emitted fluorescence at two distinct wavelengths. This ratiometric technique is however not calibration free and molecule manufacturers advise users to perform a pre-calibration using the acidic and basic endpoints of titration respectively. pH sensing is based on the monitoring of the acid-base reaction which occurs in the indicator layer grafted at the end of an optical fiber. Calibration is required to account for degradation of the sensor probe due to aging or repetitive use and because the pKa of the acid-base reaction cannot be considered constant. pKa variations are due to several factors like temperature and/or ionic strength of the solution to be measured, structure and thickness of the indicator layer at the end of the fiber. Indeed, pKa can differ from almost 2 units between the value in a low concentration solution and the value in a dense layer close to a solid surface which is the case in fiber optic pH sensors. Furthermore, it is extremely difficult to fabricate pH sensitive fibers with a reproducibility high enough to control the pKa of the acid-base reaction in the sensing volume. In this conference, we show that modeling the fluorescence properties of ratiometric indicators existing in their 2 acidic and basic forms cannot be used to access calibration free pH sensing. We then explain how pH indicators exhibiting more complex prototropic equilibria can be used to compute not only the pH value but also the value of the pKa at the moment when measurements are performed. We present the complete mathematical modeling of the fluorescence properties of fluorescein and we explain how, from any fluorescence spectrum, it is possible to fit the values of both pH and pKa. This is, to the best of our knowledge, the first example of calibration free micro pH sensor. This project has received partial funding from the European Union Horizon 2020 Research and Innovation program under Grant Agreement No 754907.

10:00-11:00 **Karsten Hinrichs**:Leibniz Institut ISAS, Germany. **Invited**
Infrared nanopolarimetric analysis of structure and anisotropy of thin films

Infrared (IR) spectroscopic techniques typically can deliver simultaneously high chemical and structural contrast. The photothermal atomic force microscope infrared-spectroscopy (AFM-IR) technique can bridge the gap between micro- and nano-scale IR spectroscopic analysis of local anisotropic material properties. The materials anisotropy plays a key role in polymer, optoelectronic and bio-related research issues. In this presentation recent progress and perspectives in IR spectroscopic nanopolarimetric analysis (about 30 nm resolution) of anisotropic thin film materials are presented. Several highly sensitive polarization dependent nano-scale analyses of polaritonic films, polymer films, bio-sensing surfaces, aggregates of large molecules and protein aggregates are discussed. The measured infrared spectra of thin films can be interpreted within analytical optical simulations involving oscillator and dispersion models in combination with numerical calculations.

Appl. Spec. 72 (2018) 817
Opt. Mater. Express 7 (2017) 3706

11:00-11:40 **Natalie Foster**:UT Austin, USA.

Strain dependence of $\chi^{(2)}$ in thin film barium strontium titanate

Ferroelectrics such as BaTiO3 are materials whose dielectric and nonlinear optical properties can be tuned to efficiently modulate light and challenge the current standard on nonvolatile memory. They exhibit strong second harmonic response attributed to a built-in polarization, which acts as a diagnostic tool in determining their success as electrooptic modulators. Through optical second harmonic generation (SHG) in reflection, we characterized variations in second order nonlinear susceptibility $\chi^{(2)}$ as a function of thickness and compressive strain in epitaxially-grown Ba1-xSrxTiO3 (BSTO) thin film alloys on lattice-mismatched SrTiO3 substrate. Spectroscopic ellipsometry showed that the BSTO dielectric function was nearly x-invariant in the range of fundamental (780 nm) and SHG (390 nm) wavelengths. We observed a peak in SHG intensity for a given film thickness around x=0.3 corresponding to a strain of about -1.7% and corroborated these results with both x-ray diffraction and high-resolution electron microscopy.

12:10-12:50 **Kjeld Pedersen**: Aalborg University, Denmark.
Optical characterization of SiC thin films on Si(111)

Thin SiC films grown on Si wafers are potential substrates for wide bandgap devices with applications in optoelectronics, power electronics, and micro-electromechanical systems. Recently a new method for growth of epitaxial SiC layers on Si has been developed where carbon atoms are substituted into the Si matrix [1]. The process leads to nucleation of SiC with a crystalline structure and orientation dictated by the original Si matrix. Such SiC films may serve as substrates for further growth of wide bandgap device layers such as nitrides or SiC by CVD processes. However, SiC appears in a large number of polytypes with different properties when used as substrates for further film growth. Furthermore, the SiC thin films on Si form columnar structures with properties that depend strongly on growth conditions. Characterization of polytypes as well as the nanocrystalline structures is therefore important in order to develop high quality device layers. In this work the effect of SiGe buffer layers introduced at the Si surface before SiC growth is investigated. Photoluminescence is expected to be weak from SiC bulk crystals due to the indirect bandgap. However, the nanocrystaline structure of the SiC layers results in enhanced exciton recombination as the small sizes can relax the selection rules. Green luminescence appearing consistently with a peak at 2.5 eV and a long low-energy tail is ascribed to the surfaces of the SiC columns of the film, possibly an oxide formed during the high temperature growth process. Luminescence in the blue and UV range indicates stacking faults with hexagonal elements included in the 3C matrix material. Very sharp UV peaks may indicate quantum confinement effects associated with the hexagonal inclusions. Optical second harmonic generation (SHG) is sensitive to the crystal structure and depends on the SiC polytype. Strong SHG signals at normal incidence show that the film is dominated by 3C SiC since the symmetry of hexagonal structures is too high to give SHG in this configuration. Azimuthal rotations of the samples demonstrate the expected 3-fold symmetry. Films grown on vicinal Si(111) substrates show a 1-fold symmetry contribution that is comparable to the 3-fold contribution, indicating that the SiC crystal aligns with Si planes. Introduction of the SiGe buffer layer increases the 3-fold contribution to the SHG signal by an order of magnitude. Since the recorded normal incidence 3-fold symmetry signal only exist as a result of cubic crystal symmetry this is a clear signature of a more well-ordered crystal structure with the SiGe buffer layer.

1. R. R. Juluri et al. Thin Solid Films 662, 103 (2018)

12:50-13:50 **Giuseppe Pirruccio**: IF, UNAM, México. **Invited**
Extended chiro-optical near-field response of achiral plasmonic lattices

We investigate the chiro-optical properties of the electromagnetic near-field associated with the excitation of collective optical resonances (surface lattice resonances) in achiral plasmonic lattices. These arrays are specially designed to support dispersive resonances with non-trivial, multipolar near-field distributions in the surroundings of the nanostructure, which in turn gives rise to an enhanced chiro-optical response. The presence of these multipolar resonances in lattices without explicitly broken mirror symmetry is experimentally confirmed by far-field extinction measurements, while the angular, spectral and spatial dependence of the associated chiral near-field are numerically simulated. Lattice resonances allow for extended, enhanced, single-handed and homogeneous near-field chiro-optical response without the need of intrinsically chiral plasmonic nanomaterials. We believe that the proposed structure can be potentially utilized as a substrate for enhanced background-free enantioselectivity and tunable chiral molecule recognition over large areas.

15:30-16:30 **Eugenio Méndez**: CICESE, México. **Invited**
Goos-Hänchen shifts in the reflection of partially coherent beams

We study the lateral displacement of specularly reflected speckle patterns and partially coherent beams from the position expected on the basis of geometrical optics. The effect, known as the Goos-Hänchen shift, which has been well studied for the case of coherent beams, is relevant in the theory of dielectric optical waveguides and may be understood in terms of the phase change acquired upon reflection at the interface by the plane waves contained in an angular spectrum representation of the incident beam. We find that the shift of a partially coherent beam depends, not on its width, as is the case of a coherent beam, but of the lateral size of the coherence patch. It is shown that, as far as the shift is concerned, one can find equivalent situations in these two cases, which depend on the relation between the beam width and the width of the coherence patch (or the speckle size). The theoretical results are illustrated and tested by means of computer simulations in situations involving the total internal reflection of optical beams at dielectric interfaces.

16:30-17:10 **Thomas Hannappel**: Ilmenau University of Technology, Germany. **Invited**
Optical in Situ Determination of the stoichiometry in GaAsP Graded Buffers During MOVPE

Epitaxial integration of direct bandgap III/V compounds on Si may use GaAsP graded buffer layers to bridge the lattice constant from GaP towards GaAs or germanium. In a new GaAsP/Si dual-junction solar cell concept utilizing strain-balanced multi-quantum wells, solar energy conversion efficiencies above 40% are feasible and GaAsP grading to only 50% of As is required. Si(100) substrate preparation as well as low-defect pseudomorphic GaP nucleation on Si(100) have been established as ideal starting point for GaAsP grading, which we study here in situ with reflection anisotropy spectroscopy (RAS). We find that the growth surface exhibits optical fingerprints of a well-ordered, group-V rich surface reconstruction. With increasing As supply, a characteristic feature in the RA spectrum which is assigned to surface-modified optical bulk transitions close to the E1 critical point energy shifts towards lower photon energies. Within a simplified empirical model, this shift depends approximately linearly on the As percentage x in the GaAsxP1-x layer (obtained by ex situ high-resolution X-ray diffraction) and it can be described in analogy to the shift of E1 from GaP to GaAs. The shift is well observable at growth temperature and for a broad range of As concentrations since both the P-rich GaP(100) surface and the As-rich GaAs(100) surface exhibit characteristic peaks at E1. The evaluation of the shift is further eased by strong absorption suppressing interference modulations. Thus, the stoichiometry of individual GaAsxP1-x layers can be quantified in situ during growth, which is beneficial for process control and optimization.

Tuesday 4

17:10-19:00 **Poster Session**

P1 Second-harmonic generation of SiC nanotubes: First principles studies
Raúl Vazquez, CIO, México

P2 Role of Van der Waals Interactions in Encapsulation of Organic Molecules into Boron Nitride Nanotubes
Raúl Vazquez, CIO, México

P3 Influence of defects on methane adsorption characteristics of MoS2: the first principle study
Jiaming Ni

P4 Dielectric function of crystalline systems with GW eigen-energies
Cristian Montes, CIO, México

P5 Second Harmonic Generation in Nanostructured Metamaterials
Ulises Meza, CIO, México

P6 Structure and optical properties of clean and functionalized Si(hhl)-Au surfaces
Conor Hogan, (ISM -CNR), Italy

P7 Graphene Oxide Composite Hydrogel fora Transdermal Delivery of Metformin
Lorena Gárate, UASLP, México

P8 Two-photon absorption spectroscopy and anisotropy of bulk III-V semiconductors and quantum dots
Brandon Furey, UT Austin, USA

P9 Theory of ab initio calculations for third order nonlinear susceptibilities focused in two photon absorption
Alan Bernal, CIO, México

P10 Second Harmonic Generation as an Optical Probe of Buried defects
Sergio Beltrán, CIO, México

P11 Optical Properties of Monolayer and Bilayer Particle-Arrays
David Becerril, IF, UNAM, México

P12 Second Harmonic Spectroscopy of InP:Si thin films
Ramón Carriles, CIO, México

P13 Creation of a Perl software for generating movies to describe metamaterials optical properties
Felix Neira, CIO, México

10:00-11:00 **Valérie Véniard**: LSI, Ecole Polytechnique, France. **Invited**

Optical nonlinear processes in semiconductors in the presence of a DC field: an ab-initio description

A deep understanding of the nonlinear optical properties of solids is crucial for the improvement of nonlinear devices and provides an opportunity to search for new materials. Among all the non-linear phenomena existing in nature, an important role is played by the electro-optic effect. The electro-optic effect produces a change of the refractive index in a medium using a DC electric field and has attracted particular interest for the development of opto-electronic devices. In the linear electro-optic effect (LEO) or Pockels effect, the change is proportional to the applied electric field. It may be seen as a second-order polarization and then described by a second-order susceptibility, which is known to be zero in the dipole approximation for centro-symmetric materials. Therefore a peculiarity of the LEO effect comes from the fact that it only occurs in materials without inversion symmetry or originates from symmetry-breaking regions.

From the theoretical point of view, most of the calculations for second-order susceptibilities have been done in the framework of Second Harmonic Generation (SHG), [1]. In that case, the frequency of the incoming field is considered as high with respect to vibrational frequencies and the lattice is kept static. Therefore, one has to evaluate only the electronic contribution, obtained directly from the optical susceptibility, coming from the interaction of the valence electrons and the electric fields. The knowledge of the electro-optic tensor implies in principle the evaluation of two additional contributions, the ionic and piezoelectric parts. The ionic contribution is linked to the ionic displacements and depends on the variation of the dielectric tensor induced by these displacements. The piezoelectric contribution comes from the possible modification of the shape of the unit cell due to the electric forces, [2]. Following the same idea, a similar phenomenon happens also for SHG, corresponding to a second harmonic response in the presence of a dc-field, called Electric Field Induced Second Harmonic (EFISH) and described in terms of a third-order polarization.

I will show our results for the second order susceptibility describing the LEO tensor, within the ab initio framework of time-dependent density-functional theory. I will present our analytic derivation of the macroscopic polarization up to second order in terms of the electric fields, including the effect of a scissors operator to account for the quasi-particle effect. Excitonic effects will be included on the basis of a simple approach, [3]. The ionic contribution will be evaluated within the same framework and included explicitly. These results will be compared with experimental data. Furthermore, while the ionic part is often evaluated through the Faust-Henry coefficient [4], the validity of this approximation will also be discussed. Preliminary results will be presented for the EFISH process.

(1) Semiconductor Science and Technology 31, 123002 (2016).
(2) Phys. Rev. B 71,125107 (2005).
(3) Phys. Rev. B 97, 205201 (2018).
(4) Phys. Rev. Lett. 17, 1265 (1966).

11:00-12:00 **Raúl Esquivel**: IF, UNAM México. **Invited**
Optics of surfaces, interfaces and their role in radiative heat transfer

In this work we present a study of the variation of the near-field radiative heat transfer as a function of the optical response of the surface of the emitting bodies. First we briefly describe the theory of fluctuating electrodynamics and its use in calculating the thermal emission in the near-field. The most important features such as the coherence in the spectral heat transfer is explained, as well as the dependence of the thermal emission with the dielectric function of the body. As case studies, we consider the case of simple polaritonic surfaces and compare the results with that of a metallic surfaces. Then, we consider an Al surface and show how the oxidation of the surface is a way of changing the heat flux. The oxidation inhibits the plasmonic modes of the surface and activates the polaritonic modes of the oxide, enhancing the near-filed heat transfer (NFHT). The combination of polaritonic and metallic materials can lead to the appearance of Fano-like resonance on the spectral heat transfer when low plasma metals like Bi are used. By tuning the plasma frequency of the metal with the transverse phonon frequency of the polaritonic material it is also possible to have thermal frequency gaps, where heat transfer is suppressed. As a final example we consider the case of metallic sponges or mesoporous materials where the porosity is used to change the heat transfer.

1. Phys. Rev. Materials (Rapid Comm.) , 00, 002200(R) (2017).
2. Phys. Rev. Materials, vol. 3, 015201 (2019).
3. J. Phys. Chem. C, 123 10598 (2019).

10:00-11:00 **Conor Hogan**: ISM-CNR, Italy. **Invited**
Phase transition and electronic structure of the antimonene/Bi_2Se_3 van der Waals heterostructure

Layer-by-layer stacks of two-dimensional materials - so called 'van der Waals heterostructures' - have attracted a great deal of interest in recent years [1]. Due to the flexibility in design, they offer potential across a wide range of applications from photovoltaics to tunneling devices. Moreover, interesting physical properties and functionalities emerge that derive from the 2D nature of the component sheets (such as charge and spin density waves, 2D excitons) and for particular heterostructures, via proximity effects (whereby one material inherits some property of another through some electronic coupling). Within this framework, the heterostructure formed between the 2D trivial semiconductor antimonene (Sb-ene) and the 3D topological insulator Bi2Se3 offers a fascinating route for exploring unconventional interfacial phenomena whereby both the trivial and topological insulator undergo stunning changes through the proximity effect [2].

1. Science 353 (2016) aac9439, Nanotech. 29 (2018) 065704
2. Phys. Rev. B 93 (2016) 075308

11:00-11:40 **David Becerril**: IF, UNAM, México.
Near-Field Energy Transfer Between Nanoparticles Modulated by Coupled Multipolar Modes

We present a study of the role of coupled surface modes in radiative energy transfer between small spherical nanoparticles mediated by multipolar interactions. We show the importance of including multipolar distributions as well as full interaction and coupling between particles at nanometer separation distances and identify the regime where the single scattering approximation is valid. We analyze how multipolar interaction affects coupled surface modes which are additional channels through which energy is transferred increasing energy transfer nearly an order of magnitude, which is commonly neglected or calculated at the dipole level only. Furthermore, it is shown that excitation of multipolar coupled modes brings about an overall broadening of the flux spectrum leading to a substantial increase of power exchange compared to the single scattering or dipole approximations. The increase of energy transfer brought about by the excitation of multipolar coupled modes at nanometric separation distances may help account for deviations observed in experiments when compared to current models. Our method employs a combination of the fluctuation-dissipation theorem and a multipolar spectral representation. This latter separates dielectric and geometric parameters of the system, allowing unambiguous identification of coupled surface modes. With this formalism, we have also studied the radiative energy transfer in a system of three particles with varying separation distance. The inclusion of multipolar interactions was used to study many-body effects at small separation distances where the dipole approximation has been typically used but is insufficient to describe full interactions. Optimal parameters for the enhancement of energy transfer, of up to an order of magnitude due to a third particle were found which were found to depend on the tendencies of the coupled modes of the system. In the trimer system heat flux spectrum is enhanced by up to two orders of magnitude for specific energies and separation distances leading to an enhancement of power exchange of up to an order of magnitude relative to the dimer.

Thursday 6

12:10-12:50 **Ricardo Tellez**: CICESE, México.

Near-field characterization of plasmonic resonances of metallic nano-structures integrated to ion-exchanged glass waveguides

The interaction of electromagnetic waves considering both, electric and magnetic fields, with structured metamaterials has been largely studied in recent years, leading to a new research field named metaphotonics. An ultimate aim is to combine different optical components into single miniature optical chips that serve as a bridge to overcome the huge size mismatch between diffraction limited microphotonics and bandwidth limited nanoelectronics. Among the large variety of integrated metaphotonic devices, plasmonic nanostructures coupled to dielectric waveguides are of particular interest because they reduce the inherent light propagation losses in metallic metamaterials, promising new applications for optical quantum communications and biosensing devices. In this contribution we show the near-field characterization of hybrid integrated photonic-plasmonic devices consisting of metallic nanostructures (strip and periodic array of nanowires) integrated on top of ion-exchanged glass waveguides. The samples were fabricated with electron beam lithography, while the characterization was performed with a near-field scanning optical microscope (NSOM). The results show that the plasmonic resonances of the nanostructures can only be excited with the fundamental TM0 mode of the waveguide and we also demonstrate that even when the periodic array of nanowires is subdiffractive, there is no coupling between the plasmonic resonances of each nanowire, hence the periodic system can be regarded as a collection of individual localized light sources. Furthermore, due to the low propagation losses, low birefringence and compatibility with optical commercial fibers of the glass waveguides, our designed structures stand as good candidates for the development of integrated metaphotonic devices operating at visible wavelengths for lab-on-a-chip applications.

Opt. Express 24 (2016) 13875
JOSA B 34 (2017) 2147
JOSA A 30 (2013) 2347

12:40-13:50 **Thomas Pedersen**: Aalborg University, Denmark. **Invited**
Excitonic Stark effect and ionization in transition-metal dichalcogenides

Semiconducting transition-metal dichalcogenides (TMDs) are characterized by unique optical properties. In their monolayer form, MoS2, MoSe2, WS2, and WSe2 are direct band gap materials with exciton binding energies reaching several hundred meVs. The exciton-ic optical response can be manipulated by external electric or magnetic fields. In this presentation, we use the Wannier exciton model to study the excitonic response in exter-nal fields [1,2]. Specifically, we compute Stark and Franz-Keldysh shifts of bound and continuum excitons. The experimental signatures of external fields are studied for a range of different TMDs in various dielectric environments. In photodetectors and solar cells, optically generated excitons must be ionized to sepa-rate electrons and holes. If the excitons are strongly bound, thermal ionization is ineffi-cient. A strong electric field, however, can greatly enhance the ionization rate. We study this process theoretically for mono- and multilayer transition-metal dichalcogenides within a modified Wannier exciton model [2]. The effects of dimensionality and screening on the exciton binding energy are discussed. In the presence of a strong electric field, the exci-ton energies become complex resonances. By applying the complex scaling techniques to Mo and W based compounds we compute the field-dependence of the ionization rate for both monolayer and multilayer photodetectors.

1. Phys. Rev. B. 94, 125424 (2016).
2. Nature Commun. 9, 1633 (2018).

Thursday 5

15:30-16:30 **Volodymyr Dzhagan**: V. Lashkaryov Institute, Ukraine. **Invited**

Phonon spectra of strongly confined chalcogenide nanocrystals: physical insights and structural information

The high flexibility of chemical routes for tailoring the properties of colloidal nanocrystals (NCs) of various metal chalcogenides (CdTe, Cu2-xS, Cu2ZnSnS4, etc.) and NC-based composites stimulates ever-growing activities in synthesis, investigation, and application [1]. Unveiling the internal structure of core-shell or other types of heterogeneous NCs (CdSe/CdS, CuInS2/ZnS, etc.) and bringing them into accord with model expectations is even more challenging than for their homogeneous counterparts. Along with varying the NC size and composition, changing the ligands on NC surface is an additional powerful way of tuning the NC properties. Different spectroscopic techniques have been employed for achieving a better understanding about the structure of the NCs and its relation with their physical and chemical properties. Here, we survey the capabilities of vibrational Raman scattering and infrared (IR) absorption spectroscopies in probing the phonon spectra and the structure of metal chalcogenides of semiconductor NCs prepared by colloidal chemistry. Vibrational Raman or IR spectroscopy of NCs can provide information on phonon modes, lattice constants, structural disorder, and strength of electron-phonon coupling [2]. Owing to the possibility of selectively probing materials having different bandgaps by using different excitation wavelengths in the Raman experiments, core/shell and other hetero-NC morphologies can be distinguished from alloyed NC formation [2]. Moreover, for multinary chalcogenide NCs like Cu2ZnSnS4 the possible formation of secondary phases (Cu2-xS, CuxSnSy, ZnS, etc) can be detected more efficiently than e.g. by X-ray diffraction. The high sensitivity of the phonon frequency to the lattice constant of a crystal allows the lattice mismatch-induced strain in core/shell NCs to be measured. Studying the size-dependence of the phonon spectra provides a characteristic NC size at which the surface starts to dominate over the structure of the parental bulk crystal. Free-standing 2D colloidal semiconductor nanocrystals, or nanoplatelets, show a number of distinct phonon features which were not observed for spherical and other NC shapes [3].

1. Chem. Rev. 116 (2016) 10513
2. J. Phys. D Appl. Phys. 51 (2018) 503001
3. Nanoscale 8 (2016) 17204

Friday 7

10:00-11:00 **W. Luis Mochán**: ICF, UNAM, México. **Invited**
Keller's theorem revisited

Keller's theorem relates the components of the macroscopic dielectric response of a binary two-dimensional composite system with those of the reciprocal system obtained by interchanging its components. We present a derivation of the theorem that, unlike previous ones, does not employ the common assumption that the response function relates an irrotational to a solenoidal field and that is valid for dispersive and dissipative anisotropic systems. We show that the usual statement of Keller's theorem in terms of the conductivity is strictly valid only at zero frequency and we obtain a new generalization for finite frequencies. We develop applications of the theorem to the study of the optical properties of systems such as superlattices, 2D isotropic and anisotropic metamaterials and random media, to test the accuracy of theories and computational schemes, and to increase the accuracy of approximate calculations.

New J. Phys. 20 (2018) 023028

Friday 7

11:00-11:40 **Eugen Speiser**: ISAS, Germany.
Vibrational properties of Au decorated vicinal Si(111) surfaces

Gold induced atomic reconstructions on flat and vicinal Si substrates offer a range of structural variations which strongly influence electronic and optical properties of the interface. The range varies from monolayer 3×3 to the (5×2) metallic triple atomic chains on flat substrates and metallic chains of different widths on the terraces of (553), (557), (775) substrates. Often, not only is the underlying main structural motif important for the properties of these systems but also ad-atoms and novel Si step edge induced elements dominate the electronic properties giving rise to their interpretations in terms of 1D physics related phenomena. The precise knowledge about the atomic structure and its interplay with electronic properties is an important requirement for these interpretations. Vibrational spectroscopy in combination with ab-initio DFT based calculations was established in the last decades as one of the methods of choice for investigation of structural and dynamical properties of surfaces and interfaces. We report on the in situ UHV Raman analysis of self-organized Au submonolayers on nominal Si(111) surfaces, as well as on vicinal Si(553), Si(775), and Si(557). The assignment of groups and individual vibrations is achieved by phenomenological comparison of spectra and matching with theoretical calculations. In this way unambiguous vibrational markers for each surface are identified and tested on mixed domain reconstructions. The tracing of these marker modes and their parameters like intensity, frequency and line shape upon the change in e.g. temperature and additional adsorptions allows to draw conclusions on structure and dynamic properties.

11:40-12:40 **Mildred Quintana**: IF, UASLP, México. **Invited**

2D Material-Metal Nanoparticle Platforms for Surface Enhanced Raman Scattering (SERS) Sensing of Polyaromatics and Biomolecules

Several methodologies have been established for the preparation of graphene and other 2D material-metal nanoparticle (NPs) hybrids towards SERS sensing platforms. In principle, 2D materials act as a substrate for the deposition or growth of NPs offering large surface areas, mechanically stable and sometimes conductive platforms. In this talk, I will summarize our recent efforts towards the functionalization and characterization of 2D material-metal NPs hybrids. I will introduce different functionalization techniques involving organic functionalization of graphene,[1] plasma doping of MoS2, and WS2,[2] and the photochemical reduction of Au NP on graphene oxide (GO).[3] We further aim to address the production of the nanohybrids towards the development of SERS sensors.[2,3] I will discuss our approach, the limitations found and the strategies followed to increase the sensitivity of devices by the synergetic effects emerging from the interaction of metal NPs and the 2D substrate.

1. R. Soc. open sci. 5 (2018) 180605
2. ACS Appl. Nano Mater. 1 (2018) 3625
3. Phys. Chem. Chem. Phys. 20 (2018) 1685