9-10 June 2022, Institute of Physics Belgrade

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WORKSHOP IN STRONGLY CORRELATED ELECTRON SYSTEMS

*Special focus of the conference will be devoted to Iron-chalcogenide superconductors and research performed during **StrainedFeSC project.***

"Workshop in strongly correlated electron systems" will be held in honor of Academician Zoran V. Popovic.

This workshop is supported by the Science Fund of the Republic of Serbia under the grant number 6062656 at Institute of Physics Belgrade Serbia.

Organization Committee

Dr. Nenad Lazarević, *Institute of Physics Belgrade, University of Belgrade*
Dr. Jelena Pešić, *Institute of Physics Belgrade, University of Belgrade*
Dr. Borislav Vasić, *Institute of Physics Belgrade, University of Belgrade*
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WORKSHOP IN STRONGLY CORRELATED ELECTRON SYSTEMS
BELGRADE, JUNE 9 – 10, 2022

CONFERENCE PROGRAMME

Thursday, June 9, 2022

10^{00} – 10^{30} Welcome speech by the director of Institute of Physics Dr. Aleksandar Bogojević

10^{30} – 11^{00} Honorary speech, Zoran V. Popović, *Serbian Academy of Sciences and Arts, Belgrade, Serbia*

11^{00} – 11^{30} **Raman scattering study of the $FeSe_{1-x}S_x$**, Nenad Lazarević, *Institute of Physics Belgrade, University of Belgrade , Belgrade, Serbia*

11^{30} – 12^{00} **Light scattering in Fe pnictides and chalcogenides**, Rudi Hackl, *IFW Dresden, Dresden, Germany*

12^{00} – 12^{30} **Spin-lattice correlations at elevated temperatures in $EuTiO_3$**, Efthymios Liarokapis, *Department of Physics, National Technical University of Athens, Greece*

LUNCH BREAK

14^{00} – 14^{30} **Symmetries of layered structures**, Božidar Nikolić, *NanoLab, Faculty of Physics, University of Belgrade, Belgrade, Serbia*

14^{30} – 15^{00} **Nanoscale resistive switching in iridates and manganites**, Borislav Vasić, *Center for Solid State Physics and New Materials, Institute of Physics Belgrade, Serbia*

15^{00} – 15^{30} **Interplay of anomalous Hall angle and magnetic anisotropy in ferromagnetic topological crystalline insulator thin films,** Rajdeep Adhikari, *Institut für Halbleiter-und-Festkörperphysik, Johannes Kepler University, Linz, Austria*

15^{30} – 16^{00} **First Principle study of Evolution of Vibrational Modes of FeSe Under Uniaxial Strain,** Jelena Pešić, *Center for Solid State Physics and New Materials, Institute of Physics Belgrade, Serbia*

16^{00} – 16^{30} **Steps towards ab-initio predictions of electron mobility in materials with strong electron-phonon interaction**, Nenad Vukmirović, *Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia*

COFFEE BREAK

16^{45} – 17^{15} **Infrared and Raman Study in narrow gap semiconductor $FeGa_3$**, Darko Tanasković, *Institute of Physics University of Belgrade, Belgrade, Serbia*

17^{15} – 17^{45} **Effective Medium Theory in Maxwell Garnett Aproximation for Structural and Optical Characterization of some Chalcogenide – based Semiconducting Nanomaterials,** Jelena Mitrić, *Institute of Physics University of Belgrade, Belgrade, Serbia*

17^{45} – 18^{15} **Suppression of superconductivity and nematic order in FeSe1-xSx ($0 \leq x \leq 1$)**, Cedomir Petrovic, *Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, USA*

Friday, June 10, 2022

10^{00} – 10^{30} **A new family of Kitaev materials,** Qingming Zhang, *Lanzhou University, Institute of Physics, Chinese Academy of Sciences, Lanzhou, Gansu, China*

10^{30} – 11^{00} Complex oxide heterostructures for efficient spin to charge conversion, Alberto Pomar, *Instituto de Ciencia de Materiales de Barcelona, Barcelona, Spain*

11^{00} – 11^{30} **DFT+Σ2 method for electron correlation effects at transition metal surfaces and nano-devices**, Miloš Radonjić, *Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia*

COFFEE BREAK

11^{45} – 12^{15} **Dynamic tuning of quantum light emission from GaN/InGaN nanowire quantum dots by surface acoustic waves**, Snežana Lazić, *Departamento de Física de Materiales, Instituto 'Nicolás Cabrera' and Instituto de Física de Materia Condensada (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain*

12^{15} – 12^{45} **First-principles exploration of superconducting 2D materials for emerging quantum technologies**, Jonas Bekaert, *Condensed Matter Theory (CMT), Department of Physics & NANOlab Center of Excellence, University of Antwerp, Antwerp, Belgium*

12^{45} – 13^{15} **The electric field gradient at ^{57}Fe in $Fe_{1-\delta}Te_2$,** Valentin N. Ivanovski, *Department of Nuclear and Plasma Physics, Vinca Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*

LUNCH BREAK

15^{00} – 15^{30} **Nonlinear and dynamic behaviour of exciton-polariton coupling processes in WS_2 nanostructures**, Bojana Višić, *Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia, Solid State Physics Department, Jozef Stefan Institute, Ljubljana, Slovenia*

16^{00} – 16^{30} **Synthesis and characterization of ternary Van der Waals MoxWx-1S2 nanotubes for advanced field emission application**, Luka Pirker, *Condensed Matter Physics Department, Jozef Stefan Institute, Ljubljana, Slovenia, Department of Electrochemical Materials, J. Heyrovský Institute of Physical Chemistry, Praha, Czech Republic*

16^{30} –17^{00} **Influence of magnetism and electron-phonon interaction on lattice dynamics of pure and Co-doped $K_xFe_{2-y}Se_2$ single crystals**, Marko Opačić, *Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia*

COFFEE BREAK

17^{15} –17^{45} **Suppression of inherent ferromagnetism in Pr-doped CeO_2 nanocrystal**, Novica Paunović, *Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia*

17^{45} – 18^{15} **Fluctuating hexamer precursor to a two-stage electronic transition in RuP**, Emil Bozin, *Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory, Upton, USA*

18^{15} ***Closing Ceremony***

Raman scattering study of the $FeSe_{1-x}S_x$

N. Lazarević[1], A. Baum[2, 3], A. Milosavljević[1], L. Peis[2, 3], R. Stumberger[2, 3], J. Bekaert[4], A. Solajić[1], J. Pešić[1], A. Wang[5], M. Šćepanović[1], M. V. Milošević[4], C. Petrovic[6], Z.V. Popović[1, 7] and R. Hackl[2, 3, 8]

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[6]*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973-5000, USA*
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A Raman scattering study of the entire substitution range of the FeSe1−xSx solid solution is presented. Experimental data were obtained as a function of temperature, scattering symmetry and sulfur concentration x ($0 \leq x \leq 1$). All excitations - phonons, spins and charges are analyzed thoroughly. The energy and width of iron-related B_{1g} phonon mode vary continuously across the entire range of sulfur substitution, whereas the A_{1g} chalcogenide mode disappears above x = 0.23 and reappears at a much higher energy when x = 0.69. Similarly, the spectral features appearing at finite doping in A_{1g} symmetry vary discontinuously. The magnetic excitation centered at approximately 500 cm^{-1} disappears for x = 0.23 and above. The low-energy mode associated with fluctuations displays maximal intensity at the nemato-structural transition and thus tracks the phase boundary.

The work was supported by the Science Fund of the Republic of Serbia, PROMIS, No. 6062656, StrainedFeSC.

Light scattering in Fe pnictides and chalcogenides

Rudi Hackl

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I will give an overview of the collaboration between the groups in Belgrade and Munich in the last 9 years since 2013. The focus will be placed on phonons in strained BaFe2As2 and frustrated magnetism in FeSe. BaFe2As2 shows a strongly direction-dependent phonon intensity which originates from the magnetic ordering. In FeSe there is no magnetic ordering down to the lowest temperatures which we interpret in terms of frustrated magnetism as a result of competing nearest and next nearest neighbor exchange interaction.

Spin-lattice correlations at elevated temperatures in $EuTiO_3$

P. Pappas[1], M. Calamiotou[2], A. Bussmann-Holder[3], and E. Liarokapis[1]

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Perovskite oxides have the tendency to show various structural instabilities with multiple ground states, ferroelectric, antiferroelectric, ferromagnetic, antiferromagnetic, skyrmion type, and complex combinations of these. During the last decade the cubic perovskite oxide $EuTiO_3$ (ETO) has attracted the scientific interest due to possible multiferroicity, hidden magnetism far above its Néel temperature (T_N=5.5K), structural instability close to room temperature, and strong spin-lattice coupling. ETO shares almost the same lattice constant with $SrTiO_3$ (STO) and the same antiferrodistortive structural phase transition, but at much higher temperature (Ts=110K for STO compared with 282K for ETO). Despite the structural phase transition below 282K, surprisingly, no Raman mode appears from those allowed at low temperatures, as it happens in STO and other related compounds. Furthermore, an epitaxial 1 μm thick ETO film grown on (001) STO substrate was found with a much wider bandgap (≈4.5eV) than the bulk and with optical properties very sensitive to small magnetic fields even close to room temperature indicating a lower than tetragonal phase. The application of an external small (<0.5T) static magnetic field appears to have substantial changes in the structural properties of ETO both in bulk or epitaxial film form, and clearly a new phase transition around 200K emerges from those results. In this presentation the findings from all these studies will be highlighted and a plausible explanation of the results will be discussed.

Symmetries of Layered Structures

Božidar Nikolić, Ivanka Milošević, Tatjana Vuković, Nataša Lazić, Saša Dmitrović, Zoran P. Popović and Milan Damnjanović*

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Due to tremendous increase of interest in layered structures need for determination of complete symmetry of system became important. Layer groups are symmetries of such structures. There are 80 sets of layer groups, each set consisting of ordinary single and double group and magnetic (gray and black-and-white) single and double groups as well. The structural properties of layer groups are used for efficient symbolic computation (by the POLSym code) of the relevant properties, real and complex irreducible and allowed (half-)integer (co-) representations in particular. Furthermore, the band (co-)representations induced from the irreducible (co-)representations of Wyckoff-position stabilizers (site-symmetry groups) are decomposed into the irreducible components (for ordinary and gray groups up to now). These, and other layer group symmetry related theoretical data relevant for physics, layered materials in particular, are tabulated and made available through the web site https://nanolab.group/layer/.

Nanoscale resistive switching in iridates and manganites

B. Vasić[a], V. Fuentes[b], Z. Konstantinović[a], and A. Pomar[b]

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[b]Instituto de Ciencia de Materiales de Barcelona, CSIC, Campus de la UAB Bellaterra, Spain

Research on resistive switching (RS) is mainly motivated by possible applications of this effect in a design of new data storage devices such as resistive random access memories. The RS can be defined as an electrically or mechanically induced change of the resistance of various thin metal-oxide films from high- to low-resistance state (HRS to LRS), or vice versa. In order to explain complex processes during RS, the nanoscale characterization is essential. For this purpose, we employed atomic force microscopy (AFM) based methods. In the first part, we present the results for the electrically induced RS in semimetallic $SrIrO_3$ thin films as a function of metal-insulator transition (MIT) which is triggered by the reduction of film thickness [1, 2]. Thick films are semimetallic, so the transition from HRS to LRS is characterized with a smooth increase of the current without a threshold voltage. On the other hand, MIT is triggered in thin films which are therefore insulating and characterized by hysteretic I-V curves. The threshold voltage indicating the transition from high- (HRS) to low-resistance state (LRS) is well defined implying a band gap opening due to MIT. In the second part, we present results for the mechanically induced switching of surface electrical properties of $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) thin films [3]. It is demonstrated that a local pressure applied by the AFM tip leads to a drop of the electrical conductivity, finally inducing an electrically insulating state for high enough normal load. Subsequent electrical characterization by conductive AFM and Kelvin probe force microscopy indicates that the switching process is mainly governed by the flexoelectric field induced at the sample surface.

Interplay of anomalous Hall angle and magnetic anisotropy in ferromagnetic topological crystalline insulator thin films

R. Adhikari

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The interplay of conservation and breaking of local and global symmetries in topological phases of matter leads to the emergence of topological phenomena including quantum anomalous (QAH) Hall effect, topological superconductivity, and non-Abelian quantum statistics. Among the topological materials, magnetically doped topological crystalline insulators (TCI) were foreseen to host topologically protected QAH states generating multiple dissipationless edge and surface conduction channels with Chern number C >1. The symmetry protected topological phase of the SnTe class of TCI is characterized by a mirror symmetry resulting in topological surface states. Theoretical and experimental studies demonstrated that four Dirac points are located at the time-reversed-invariant-momentum (TRIM) points for the (111) plane in the SnTe compounds. In this talk, I will review the state-of-the-art of magnetically doped TCI and present our work on the electronic and magnetic properties of Sn1-xMnxTe (111) thin epitaxial layers, unraveled by means of low-T/high-μ0H magnetotransport measurements. While a spin mediated magnetoconductance is observed in layers with x≥0.03, the appearance of a hysteretic magnetoconductance behavior and of the fingerprints of square-like anomalous Hall effect,t point at the onset of a hole mediated ferromagnetic ordering for x≥0.06. The anomalous Hall angle θ_AH~0.3 determined for Sn0.92Mn0.08Te is one of the highest recorded for magnetic topological quantum materials. The tuning of the global band topology by magnetic doping opens wide perspectives for topology driven quantum spintronic technology.

First Principle study of Evolution of Vibrational Modes of FeSe Under Uniaxial Strain

Jelena Pešić and Andrijana Šolajić

Center for Solid State Physics and New Materials, Institute of Physics Belgrade, Serbia

Application of strain is one of the effective ways to engineer the various properties of materials. Iron-based superconductors are suitable materials to study the strain dependence of physical properties because their high sensitivity to variations in the local crystal structure. Among the iron-based superconductor family, FeSe is prominent example of the interplay between superconductivity, magnetism, and electronic nematicity, which can be tuned both by chemical substitution and application of physical pressure.

Here we present the first principle study of evolution of vibrational modes of the strained FeSe superconductor. We performed systematic computational study on bulk FeSe crystals with applying in-plane uniaxial strain ranging from -1.5% to 1.5% using density functional theory formalism. We focus on the effect of the straining of the lattice constant, and consequent symmetry distortion, on characteristic A_{1g} and B_{1g} modes of FeSe. These findings are to be compared with experimental data from Raman measurements studying the trend of changes of A_{1g} and B_{1g} modes with applied strain.

The work was supported by the Science Fund of the Republic of Serbia, PROMIS, No. 6062656, StrainedFeSC.

Steps towards ab-initio predictions of electron mobility in materials with strong electron-phonon interaction

Nenad Vukmirović

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Charge carrier mobility is one of the most important physical quantities for the description of any semiconducting material. In clean semiconducting materials, the mobility is fully determined by the interaction of electrons with phonons. However, there are still significant challenges to predict the mobility of the material with a known crystal structure. On the one hand, it is challenging to construct the Hamiltonian of interacting electrons and phonons at a sufficiently dense grid of electron and phonon momenta and subsequently evaluate the mobility within the perturbative approach based on the Boltzmann transport equation. On the other hand, electron-phonon interaction can be rather strong so that polarons are formed and the perturbative approach is not applicable. We review here our efforts aimed at overcoming both of these challenges.

We present first our results for the mobility of conduction band electrons in II-VI semiconductors ZnSe, CdTe, ZnTe and CdSe [1]. Temperature dependence of mobility was calculated using an ab-initio methodology, where electronic bands, phonon bands and electron-phonon coupling constants were obtained from density functional theory calculations. Fourier-Wannier interpolation procedure was performed to obtain these quantities on a dense momentum grid which is necessary to obtain reliable values of these quantities. Density functional theory calculations were performed using the ABINIT code, while Fourier-Wannier interpolation and final calculation of the mobility was performed using our in-house parallel code. The results indicated that mobilities obtained from calculations within generalized gradient approximation to density functional theory overestimate the experimental mobility several times. Very good agreement with experiments was obtained when electronic band structure and high-frequency dielectric constants were obtained using the hybrid HSE06 functional. We also identified simpler models that can yield accurate predictions of the mobility without using the full procedure for interpolation to a dense momentum grid.

Next, we present our development of the methodology for the calculation of charge carrier mobility in the systems with local electron-phonon interaction of arbitrary strength [2]. The method is based on unitary transformation of the Hamiltonian to the form where the nondiagonal part can be treated perturbatively. The mobility was subsequently evaluated from Kubo's linear response formula. The methodology was applied to investigate the carrier mobility within the one-dimensional Holstein model for a wide range of electron-phonon coupling strengths and temperatures. The results indicated that for low electron-phonon coupling strengths the mobility decreases with increasing temperature, while for large electron-phonon coupling the temperature dependence can exhibit one or two extremal points, depending on the phonon energy.

[1] N. Vukmirović, Phys. Rev. B 104, 085203 (2021).
[2] N. Prodanović and N. Vukmirović, Phys. Rev. B 99, 104304 (2019).

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Infrared and Raman Study in narrow gap semiconductor $FeGa_3$

C. Martin,[1] V. A. Martinez,[2] M. Opačić,[3] S. Djurdjić-Mijin,[3] P. Mitrić,[3] A. Umićević,[4] V. N. Ivanovski,[4] A. Poudel,[1] I. Sydoryk,[1] Weijun Ren,[5] R. M. Martin,[6] D. B. Tanner,[2] N. Lazarević,[3] C. Petrovic,[5] and D. Tanasković[3]

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Intermetallic narrow-gap semiconductors have been intensively explored due to their large thermoelectric power at low temperatures and a possible role of strong electronic correlations for their thermodynamic and transport properties. Here we study the optical spectra and vibrational properties of a single crystal of $FeGa_3$. The optical conductivity obtained from reflectance measurements indicates an indirect energy gap of around 0.4 eV in agreement with DFT calculations and resistivity measurements. A precise determination of the gap is hindered by a substantial spectral weight below 0.4 eV. The appearance of these in-gap states is consistent with measured non-monotonic resistivity in $FeGa_3$. The infrared and Raman spectra appear below the in-gap spectral weight. Their frequen- cies are in excellent agreement with our DFT calculations. The frequency temperature dependence is weak between 4 and 300 K, implying the absence of any phase transition. Most of the infrared and Raman lines are very narrow due to just a small number of charge carriers available for phonon scattering in this insulating compound. The Mössbauer lines that we measured are very narrow which also indicates a high quality of the single crystal.

Effective Medium Theory in Maxwell Garnett Aproximation for Structural and Optical Characterization of some Chalcogenide – based Semiconducting Nanomaterials

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In this work synthesis, as well as structural and optical properties of four chalcogenide semiconducting nanomaterials representatives were presented: europium doped gadolinium – zirconate, with chemical formula $Gd_2Zr_2O_7$ and yttrhrium – vanadate, YVO_4 and cadmium – telluride, CdTe. For synthesis of these four materials three methods were used: solution combustion synthesis for $Gd_2Zr_2O_7$, solution combustion synthesis and classical ceramics method for YVO_4 and thermal evaporation method for CdTe. The goal of this work is to register and describe different nanoobjects in prepared nanomaterials and to explain the impact of reduced dimensions on structural and optical properties of semiconducting nanomaterials using mostly Infrared and Raman spectroscopy. For complete charactrization, X – ray diffraction, Scanning Electron Microscpy and Atomic Force Microscopy were used. For analysis of gadolinium – zirconate in infrared part of the electromagnetic spectrum, theory of effective medium in Maxwell Garnett aproximation was used in order to register electron – phonon interaction which explains the shifted modes of reflectance spectra of $Gd_2Zr_2O_7$ nanopowders in comparison to bulk $Gd_2Zr_2O_7$. Low frequency modes were assigned for the first time following the rules of isotope effect. Also, optimal conditions for two crystal phases of $Gd_2Zr_2O_7$, ordered pyrochlore and disordered fluorite, were established. For yttrium – vanadate, isotope effect was applied to explain the incorporation of europium ions in yttrium – vanadate lattice and its effect to Raman spectra. The detailed calculation of shifted modes was presented, as well as comparison of two methods of preparation. Maxwell Garnett approximation was used to model its Infrared spectra and register surface optical phonons as well as some multiphonon processes. Applying effective medium theory in Maxwell Garnett approximation in CdTe thin films, the surface optical phonon – plasmon interaction was registered. This interaction originates from reduced dimension of bulk CdTe. Numerical model for calculating the reflectivity coefficient for system which includes films and substrate has been applied.

Suppression of superconductivity and nematic order in FeSe1-xSx ($0 \leq x \leq 1$)

Cedomir Petrovic

Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory

The connection between superconducting and competing order with crystalline disorder is of interest in many superconducting materials. Copper oxide materials feature a dome of superconductivity and a rather complex phase diagram with various forms of symmetry breaking orders, such as spin-density, CDW or nematic order [1]. In this talk I will discuss Fe1-ySe1-xSx ($0 \leq x \leq 1$, $y \leq 0.1$) crystals where, in contrast to copper oxides, simple crystal structure allows for clear insight into crystallographic disorder and where nematic (Ts) and superconducting (Tc) transition temperature show interesting correlation with disorder-related observables [2,3]. References: [1] E. Fradkin et al., Rev. Mod. Phys. 87, 457 (2015), [2] Aifeng Wang et al., under review (2022), [3] Aifeng Wang et al, under review (2022).

A new family of Kitaev materials

Qingming Zhang

Lanzhou University, Institute of Physics, Chinese Academy of Sciences

Kitaev spin liquid (KSL) is of fundamental significance in condensed matter physics and may lead to promising applications in fault-tolerant topological quantum computation. Just a few KSL candidates have been reported so far. Here we reveal a new rare-earth based KSL family with a high symmetry of R-3m and an undistorted honeycomb spin lattice. The strong spin-orbit coupling outputs highly anisotropic exchange interactions required by the Kitaev model. And the family shows a true two-dimensionality guaranteed by van der Waals interlayer coupling. In this talk we will introduce the fundamental magnetic properties of the family, with emphasis on YbOCl single crystals. The family offers an inspiring platform for the exploration of KSL physics and its applications.

Complex oxide heterostructures for efficient spin to charge conversion

Alberto Pomar

Instituto de Ciencia de Materiales de Barcelona, ICMAB-CSIC, 08193 Spain

The electrical manipulation of the magnetic moment of a ferromagnetic material is of vital importance for spintronic devices, aiming to store, transmit an process information while improving energu efficiency. One of the most promising techniques is the spin orbit torque that uses spin-orbit coupling to generate a pure spin current. The efficiency of spin-charge conversion is measured through the spin Hall angle. In this work, we will review our experimental results on using transition metal oxides as spin-Hall materials. We will show the succesful fabrication of all-oxide devices with efficient spin to charge conversion. We will discuss the capabilities of different perosvkite-based oxides (manganites, iridates, ...) as building blocks in spintronic heterostructures and how their physical performances may be tuned through careful control of the growth mechanisms and conditions.

DFT+Σ2 method for electron correlation effects at transition metal surfaces and nano-devices

M. M. Radonjic[1], A. Droghetti[2], A. Halder[2], I. Rungger[3], L. Chioncel[4]

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We present a computational approach for electronically correlated metallic surfaces, interfaces and two-terminal devices. The method combines density functional theory (DFT) and dynamical mean- field theory (DMFT) using a multiorbital perturbative solver for the many-body problem. Our implementation is designed to describe the electronic properties of ferromagnetic metallic thin filmson a substrate and the electronic and linear-response transport properties of two-terminal nanoscale devices and hetero-structures. Capabilities and performances are assessed in detail for two prototypical nanoscale systems.
Firstly, we compare the calculation of a Fe monolayer on a W(110) substrate with the photoemission experimental data. Our method displays significant qualitative and quantitative improvements in the spectral function with respect to the results of density functional theory within the local spin density approximation. In particular, the spin splitting of the *d* states drastically reduces, and at the same time, their spectral width becomes narrower.
Secondly, we apply the method to the metallic junctions presenting alternating Cu and Co layers, exhibiting spin-dependent charge transport and giant magnetoresistance (GMR) effect. The electron-electron correlations on the Co *d* orbitals strongly suppress coherent transmission below the Fermi level due to finite lifetime. The transmission above the Fermi level is slightly reduced since it is mostly determined by *s* electrons. At the Fermi energy, in accordance with the Fermi- liquid behaviour, the reduction of the transmission predicted by DMFT is entirely due to the shiftsof the energy spectrum induced by the electron correlations. Consequently, the resulting change in the transmission and GMR is only moderate.

References:

[1] A. Droghetti, M. M. Radonjić, A. Halder, I. Rungger, and L. Chioncel, Phys. Rev. B **105**, 115129 (2022).
[2] A. Droghetti, M. M. Radonjić, A. Halder, L. Chioncel, and I. Rungger, arXiv:2201.13118 (2022)

Dynamic tuning of quantum light emission from GaN/InGaN nanowire quantum dots by surface acoustic waves

Snežana Lazić

Departamento de Física de Materiales, Instituto 'Nicolás Cabrera' and Instituto de Física de Materia Condensada (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain

Efficient production and manipulation of single-photons are crucial prerequisites for quantum light applications. Future on-chip quantum photonics requires controllable quantum emitters that can be operated on-demand and with the possibility of in situ control of the photon emission wavelength and its polarization state. Among various non-classical light sources available, quantum dots (QDs) outdo with their integrability into existing semiconductor technologies.

Here, we report the first proof-of-principle demonstration of the dynamic real-time control, using radio frequency surface acoustic waves (SAWs), of the optical emission from QDs embedded in epitaxially grown core-shell GaN/InGaN nanowire (NW) heterostructures [1]. The SAWs are excited on the surface of a piezoelectric $LiNbO_3$ crystal equipped with an acoustic delay line onto which the NWs were mechanically transferred [2,3].

Luminescent QD-like exciton localization centers, induced by indium content fluctuations within the InGaN nanoshell, are identified using spatially, polarization- and time-resolved stroboscopic micro-photoluminescence (μ-PL) spectroscopy. They exhibit narrow and highly linearly polarized emission lines in the μ-PL spectra and a pronounced antibunching signature of single-photon emission in the photon correlation experiments [2,3]. Depending on their location within the InGaN nanoshell, nonpolar (m-), semipolar (r-) or polar (c-facet) QDs are discerned, thereby making these NWs the first single nanostructures able to host non-classical light emitters with both high- as well as low-polarity crystallographic orientations [1]. Owing to their shorter radiative lifetimes resulting from weak built-in electric field values along the growth axis, the III-nitride QDs grown on alternative low-polarity crystallographic planes are greatly beneficial for future high-speed quantum information technologies.

When such NWs are perturbed by the propagating SAW, the embedded QDs are periodically strained and their excitonic transitions are dynamically modulated by the acousto-mechanical coupling, giving rise to a spectral fine-tuning within a ~2 meV bandwidth (Fig. 1(a,b)) at the acoustic frequency of ~330 MHz [2,3]. This outcome is further combined with spectral detection filtering for temporal control of the emitted photons [2]. In this way, both spectral tunability and on-demand emission of single photons is achieved simultaneously. Moreover, the SAW-triggered acousto-electric effect inflicts changes in the QD charge population and its optical polarization [3]. Reduction (up to 30%) in the initially high linear polarization degree is observed (Fig. 1(c)). This is an important advance since, to date, the photon polarization state of III-

nitride QDs has been either probabilistic or pre-determined by electronic properties of the system.

Altogether, this study opens the door to the use of sound for scalable integration of III-nitride-based quantum emitters in nanophotonic and quantum information technologies. The advantage of the acousto-optoelectric over other control schemes is that it allows in-situ manipulation of the optical emission properties over a wide frequency range (up to GHz frequencies).

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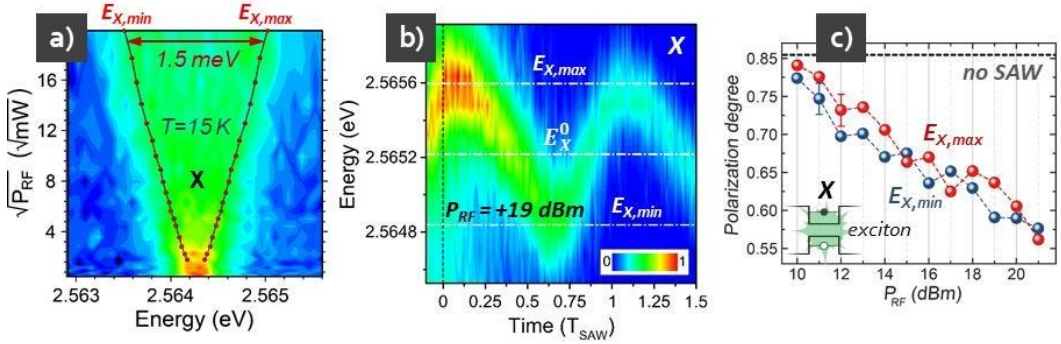
Figure 1. False color plot showing **(a)** splitting of the QD exciton (X) PL line as a function of the SAW power (Prf) and **(b)**



time-resolved (horizontal axis) normalized X PL intensity decay as a function of the emission energy (vertical axis). **(c)** Acoustically induced reduction of the optical polarization degree measured at SAW phases corresponding to the maximum tensile (E_{min}) and compressive (E_{max}) strain.

First-principles exploration of superconducting 2D materials for emerging quantum technologies

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Superconducting materials take a leading role in emerging quantum technologies, owing to their dissipation-free charge transport, which promotes quantum coherence required for many applications. For example, the largest-scale integrated quantum computing systems achieved to date are predominantly based on superconducting Josephson junction qubits [1,2]. Currently, these junctions usually consist of two bulk superconductors (e.g., Al), separated by an amorphous AlOx buffer layer. However, this system is prone to defects and roughness at the interfaces, which can strongly limit the effective quantum coherence.

Hence, alternatives are currently starting to be explored, such as van der Waals heterostructures of superconducting two-dimensional (2D) materials, separated by another insulating 2D material, or alternatively the van der Waals gap itself. Due to their atomically sharp interfaces, these systems promise enhanced qubit coherence, in combination with a capability for advanced tunability (by applying strain, gating, etc.).

To advance the development of such novel superconducting devices, extensive exploration of new superconducting 2D materials is paramount. To this end, we have performed high-throughput first-principles exploration of superconductivity in several 2D material families, such as transition metal carbides and nitrides (MXenes) [3], metal borides (MBenes) [4], and elemental monolayer materials (e.g., gallenene) [5], considering a large variety of chemical constituents. Based on our density functional theory (DFT) calculations of the electronic and vibrational properties, and the electron-phonon coupling, we solve the anisotropic Eliashberg equations to obtain the superconducting gap distribution and the critical temperature of these monolayer materials [3-5]. Therefore, our first-principles exploration yields new pathways to optimize superconductivity in the atomically-thin limit, to meet the requirements of emerging quantum technology applications.

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The electric field gradient at ^{57}Fe in $Fe_{1-\delta}Te_2$

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Transition metal dichalcogenides afford favourable physical properties which make them interesting for fundamental studies and for applications. Marcasite-type of iron ditelluride can crystallize in *Pnnm* space group with iron vacancy defects. The electric field gradient is one of the most susceptible observables for detecting changes in the charge density. Its measurements provide insight into the structure order and electronic structure of material. The goal of this talk is to approach the study of hyperfine interactions at ^{57}Fe in $Fe_{1-\delta}Te_2$ by means of Mössbauer spectroscopy along with density functional theory calculations.

Nonlinear and dynamic behaviour of exciton-polariton coupling processes in WS_2 nanostructures

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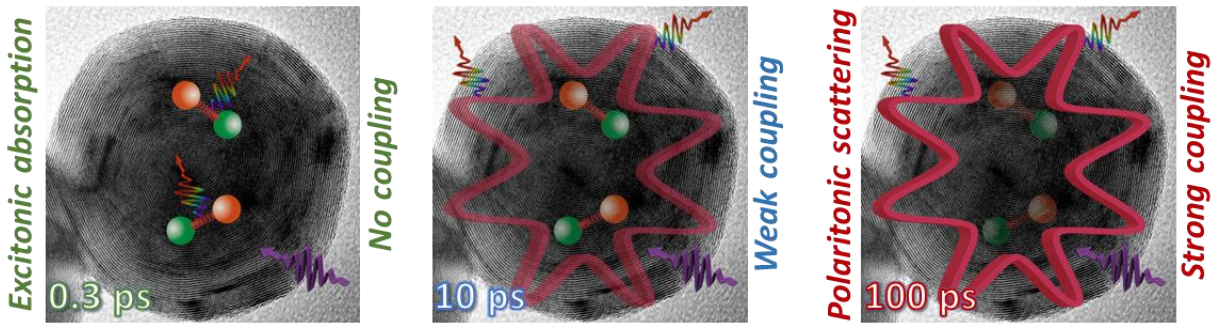
Semiconducting transition metal dichalcogenides can be synthesized in a wide range of structures and geometries, including closed cage nanostructures, such as nanotubes or fullerene-like nanoparticles (NSs). The latter are especially intriguing due to their stability, enhanced light-matter interactions, and ability to sustain exciton-polaritons (EPs) in ambient conditions, i.e., strong coupling of excitonic resonances to the optical cavity.
Here we investigate the dynamics of EPs formation in WS_2 NPs in the time domain using femtosecond transient extinction spectroscopy. We develop various analytical methods and models with time-dependent parameters to extract the underlying non-equilibrium dynamics of EPs formation. We find that the formation of EPs in WS_2 NPs is not instantaneous but a gradual process that occurs only after several picoseconds. Specifically, for the short delay times, the light-matter interaction is guided by excitonic absorption, whereas for the long delay times, the process is controlled by polaritonic scattering. We discover that the coupling strength is a time-dependent entity and not a constant as is usually defined. Namely, there is a nonlinear coupling between excitonic and external modes and a notable transition from weak to strong coupling limit. Our results show that the time-dependent phenomenological dynamical model quantitatively reproduces the nonlinear dynamical coupling as well as the effects of the pump fluence on the coupling strength.



Synthesis and characterization of ternary Van derWaals $Mo_xW_{x-1}S_2$ nanotubes for advanced field emission application

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Low-dimensional Van der Waals materials, based on atomically thin sheets stacked together, have in recent years become a rapidly developing field. Prepared from layered compounds, such as transition metal dichalcogenides (TMDCs), their constituents are held together by weak van der Waals forces. They can be found in form of quantum dots (0D), nanotubes (1D), and monolayers (2D), with eachmorphology having a unique set of properties. Their properties can be further altered by constructing heterostructures or with the synthesis of TMDC alloys.
Here we present the first $Mo_{1-x}W_xS_2$ nanotubes synthesized by the chemical transport reaction. The synthesized material has been characterized with AFM, KPFM, SEM, TEM, EDS, XRD, and Raman spectroscopy. The starting material contained MoS_2 and WS_2 in 50:50 atomic ratio. The transported material was composed of flakes and nanotubes of $Mo_{1-x}W_xS_2$. The diameters of the nanotubes range from 10 nm up to a few microns, and their length up to several 10 □m. EDS data revealed that both transition metals are homogeneously distributed in this ternary compound, but the atomic ratio is close to 60:40. TheRaman spectra of the $Mo_{1-x}W_xS_2$ NTs is a superposition of Raman peaks attributed to MoS_2 and WS_2. All of the nanotubes are multi-walled and are highly crystalline with a low number of defects. The layers growin pairs, which is the consequence of the 2H phase. The average work function of the nanotubes is around 4.7 eV, situated between the work function of MoS_2 and WS_2. Single nanotube field emission devices were prepared with two different geometrical setups. The current-voltage-behaviour of both show a linear I-V dependence and no deviations from the ideal FN behaviour.

Influence of magnetism and electron-phonon interaction on lattice dynamics of pure and Co-doped $K_xFe_{2-y}Se_2$ single crystals

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In this work, we aimed to determine the effects electronic and magnetic degrees of freedom have on vibrational properties of pure and cobalt-doped $K_xFe_{2-y}Se_2$ single crystals. Vibrational properties were investigated using Raman spectroscopy, with the help of density functional theory (DFT) calculations. Phonon spectra of superconducting $K_xFe_{2-y}Se_2$ and nonsuperconducting $K_{0.8}Fe_{1.8}Co_{0.2}Se_2$ crystals reveal Raman modes originating from metallic/superconducting *I4/mmm* phase and Fe vacancy-ordered, insulating *I4/m* phase. Temperature dependence of energy and linewidth of phonons from the insulating phase can be well described by taking into account lattice thermal expansion and anharmonicity. However, energy of the A_{1g} mode, originating from the *I4/mmm* phase, exhibits sudden hardening in the superconducting sample around critical temperature, suggesting the change of the electronic structure. By doping $K_xFe_{2-y}Se_2$ with cobalt, Raman modes from the insulating phase gradually disappear, and broad asymmetric structure become observable, probably originating from strong crystalline disorder. Raman spectra of $K_xCo_{2-y}Se_2$ single crystal host only two modes, excluding the possibility of ordered vacancies, unlike its Fe-counterpart. Ferromagnetic phase transition leaves clear fingerprint on temperature dependence of phonon energies and linewidths.

Suppression of inherent ferromagnetism in Pr-doped CeO_2 nanocrystals

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Diluted magnetic oxides are an active field of research, since they challenge our understanding of the ferromagnetism. Among the rare-earth oxides, nanostructured cerium oxide (CeO_2) has emerged as one of the most interesting oxides due to its exceptional properties which make it useful for various applications. These applications of nanocrystalline CeO_2 mostly stem from its remarkable oxygen-storage capability especially pronounced on particle surface, i.e., ability to absorb oxygen in oxygen-rich and release oxygen in oxygen-poor environment without changing its fluorite structure. The $Ce_{1-x}Pr_xO_{2-\delta}$ ($0 \leq x \leq 0.4$) nanocrystals were synthesized by self-propagating method and thoroughly characterized using X-ray diffraction, Raman and X-ray photoelectron spectroscopy and magnetic measurements. Undoped CeO_2 nanocrystals exhibited intrinsic ferromagnetism at room temperature. Despite of increased concentration of oxygen vacancies in doped samples, the results showed that ferromagnetic ordering rapidly degrades with Pr doping. The suppression of ferromagnetism can be explained in terms of different dopant valence state, different nature of vacancies formed in Pr-doped samples and their ability/disability to establish ferromagnetic ordering.

Fluctuating hexamer precursor to a two-stage electronic transition in RuP

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States of broken symmetry arising in response to Fermi surface instabilities are pivotal to emerging quantum orders. Whether such states appear coincident to global symmetry reduction, or preform away from ordered regimes underpins the underlying mechanisms. This talk focuses on detection of high temperature precursor local symmetry breaking in RuP, one of the parents of superconducting binary ruthenium pnictides, revealed by combined nanostructure sensitive powder and single crystal X-ray total scattering. Large local Ru6 hexamer distortions associated with bond-charge trimerization lift an apparent degeneracy, at the Fermi level, of flat Ru 4dxy orbital derived bands assumed to be protected by the nonsymmorphic global symmetry above the two-stage electronic transition in RuP. Implications of the precursor state for the properties of binary ruthenium pnictides will be addressed.