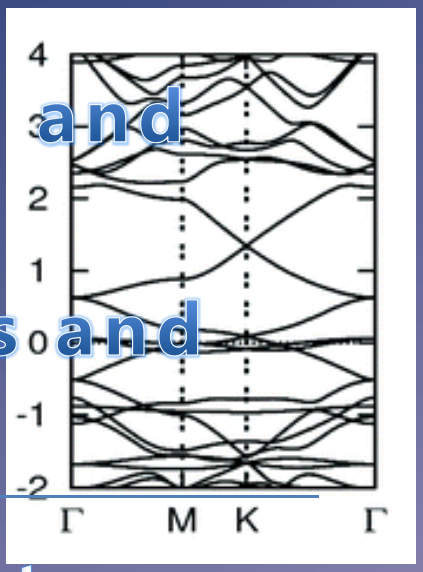
2DCP 2019, Tbilisi, Georgia

International School and Workshop on Two-Dimensional Crystals and Photonics



Program and abstract Booklet

IVANE JAVAKHISHVILI
TBILISI STATE UNIVERSITY

International School and Workshop on Two-Dimensional Crystals and Photonics

2DCP 2019

Tbilisi, Georgia

September 09-14, 2019

Ivane Javakhishvili Tbilisi State University

Faculty of Exact and Natural Sciences

International School and Workshop on Two-Dimensional Crystals and Photonics

2DCP 2019

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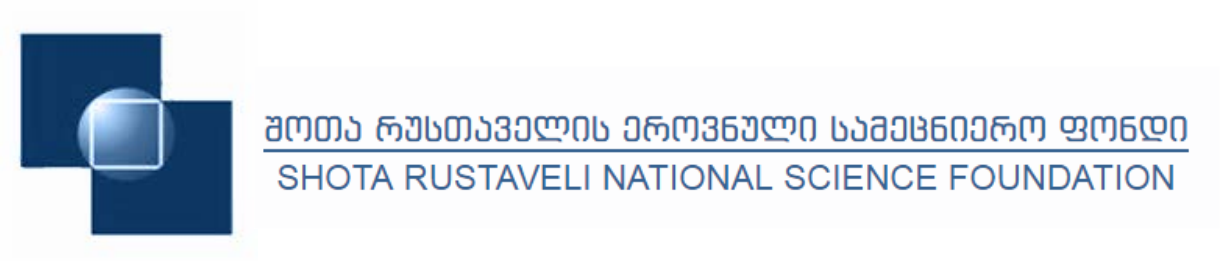

INTERNATIONAL SCHOOL ON
TWO-DIMENSIONAL CRYSTALS AND PHOTONICS

Tbilisi, Georgia | September 9-14, 2019

INVITED SPEAKERS

Baumberg Jeremy
Cambridge University - UK
Strong Light-Matter Interactions in Hybrid Plasmonic Nanostructures

Boltasseva Alexandra*
Purdue University - USA
2D Plasmonics and Metasurfaces: Fabrication and Characterization

Caldwell Joshua
Vanderbilt University - USA
Controlling Light with Nanoscale Precision with Polaritons

Finley Jonathan
TUM - WSI - Germany
Exciton-Polariton Phenomena in Complex Hybrid Nanostructures

Fogler Michael*
UCSD - USA
Hydrodynamical Models in quasi-2D Plasmonics

García de Abajo Javier
ICFO - SPAIN
Plasmons in atomically thin materials

Gumbs Godfrey
CUNY - USA
Charge Fractionalization without Electron-Electron Interaction in Bilayer Silicene

Hawrylak Pawel
University of Ottawa - Canada
Excitonic Complexes in Semiconductor and Graphene Quantum Dots

Höfling Sven
University of Würzburg - Germany
University of St Andrews - UK
Polariton Condensates in Hybrid quasi-2D semiconductors

Högele Alexander
LMU - Germany
Cavity and Magnetic Field Effects on Interlayer Excitons

Kavokin Alexey
Westlake University - China
Exciton-Mediated Supeconductivity

Lozovik Yuri
Troitsk Research Center - Russia
Superfluidity and BEC in Novel 2D Materials

Khurgin Jacob
Johns Hopkins University - USA
Waveguiding and Second Order Nonlinearities in Transition Metal Dichalcogenides

Rontani Massimo
CNR NANO - Italy
Many-Body Excitonic Effects in Low-Dimensional Quantum Systems

Shalaev Vlad*
Purdue University - USA
Trans-Dimensional Metaphotonics

Shengelaya Alexander
TSU - Georgia
Unexpected Magnetism in Semiconducting Transition Metal Dichalcogenides

Snoke David
University of Pittsburgh - USA
Exciton-Polariton Condensates in quasi-2D Microcavities

Tomanek David
Michigan State University - USA
Magic with 2D semicondutors

Ziegler Klaus
University of Augsburg - Germany
Physics of Excitons in Semiconductor Double Layers Beyond the Mean-Field Approximation

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* to be confirmed

2DCP

International School on Two-Dimensional Crystals and Photonics

- 2D Plasmonics and Metasurfaces
- Physics of Excitons in Low-Dimensional Semiconductors
- Polaritonics and Nonlinear Optics with Quantum Materials



The school includes lectures and seminars by recognized international speakers

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Michigan State University - USA
Tuning the Electronic Structure of Few-Layer 2D Semiconductors by Strain, Shear and Twist

* to be confirmed

WHERE
TBILISI, GEORGIA

Tbilisi is the capital and the largest city of Georgia, lying on the banks of the Kura River with a population of approximately 1.5 million people. Historically, Tbilisi has been home to people of multiple cultural, ethnic, and religious backgrounds and was founded over 1500 years ago.

EXCURSION
KAKHETI

In September the harvesting of grapes starts and visitors are able to acquaint with ancient tradition of winemaking. The main wine producing region of Georgia, KAKHETI, is located quite close to Tbilisi and is famous with the sightseeings and historical monuments.

VENUE
TBILISI STATE UNIVERSITY

Javakhishvili Tbilisi State University, which is the first-ever national university in the Caucasus was opened in 1918 laying the foundation for a European-type higher school in Georgia, based on Georgian educational traditions. Nowadays TSU is one of the largest higher educational institutions by its scales and it has been ranked among the top 5 percent of universities in the world, according to the Times Higher Education World University Rankings 2018.

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INTERNATIONAL SCHOOL AND WORKSHOP ON 2D CRYSTALS AND PHOTONICS

September 9-13, 2019, Tbilisi State University, Tbilisi, GEORGIA

OPENING Monday @ 8:45	MONDAY (Sep 9)	TUESDAY (Sep 10)	WEDNESDAY(Sep11)	THURSDAY (Sep 12)	FRIDAY (Sep 13)
9:00 – 10:15	L1: Tománek	L5: Finley	*FULL-DAY BUS EXCURSION TO KAKHETI (Lunch provided)*	L9: García de Abajo	L13: Ziegler
10:15 – 10:35	*Coffee Break*			*Coffee Break*	
10:35 – 11:50	L2: Höfling	L6: Högele		L10: Caldwell	L14: Shengelaya
11:50 –12:00	*Break*			*Break*	
12:00 – 12:45	S1: Benimetskiy	S3: Tsiklauri		S5: Casalis de Pury	S7: Moskalenko
12:45 – 13:45	*Lunch*			*Lunch*	
13:45 – 15:00	L3: Lozovik	L7: Rontani		L11: Stockman	L15: Kavokin
15:00 – 15:10	*Break*			*Break*	
15:10 – 16:25	L4: Snoke	L8: Hawrylak		L12: Khurgin	15:10 – 15:55 S8: Kereselidze
16:25 – 16:45	*Coffee Break*			*Coffee Break*	15:55 – 16:15 *Coffee Break*
16:45 – 17:30	S2: Berman	S4: Jaskólski		S6: Bondarev	16:15 – 17:00 *Round-Table/Poster Student Competition Awards + CLOSING REMARKS*
17:30 – 17:40	*Break*			*Break*	
17:40 – 18:30	*STUDENTS+EXPERTS Round-Table Session*	*STUDENTS+EXPERTS Round-Table Session*		*STUDENTS+EXPERTS Round-Table Session*	
18:30 – …	*WELCOME RECEPTION*	*POSTER SESSION + Career Development in Materials Science Briefing*		*GALA-DINNER*	

A. LECTURE/SEMINAR PROGRAM (speaker's last name alphabetical order)

TOPIC	INVITED LECTURE (75 min)	SEMINAR TALK (45 min)
2D Plasmonics and Metasurfaces	1. **Josh Caldwell, Vanderbilt U., USA:** Controlling Infrared Light with Nanoscale Precision Using 2D Material Polaritons 2. **F. Javier García de Abajo, ICFO, Barcelona, Spain:** Plasmonics in Two-Dimensional Crystals 3. **Alexander Shengelaya, TSU, Georgia:** Unexpected Magnetism in Semiconducting Transition Metal Dichalcogenides	1. **I.Bondarev, NCCU, USA:** Strongly Correlated Collective Excitations in Quasi-2D Nanostructures of Metals and Semiconductors 2. **A.Casalis de Pury, U. Cambridge, UK:** Plasmonic Nanoparticle Reflectors for hBN Planar Microcavities
Physics of Excitons in Low-Dimensional Semiconductors	1. **Jon Finley, TUM-WSI, Munich, Germany:** Trapping Excitons in Monolayers and Heterostructures of Atomically-Thin Semiconductors 2. **Pawel Hawrylak, U. Ottawa, Canada:** Excitonic Complexes in Semiconductor and Graphene Quantum Dots 3. **Alexander Högele, LMU, Munich, Germany:** Cavity and Magnetic Field Effects on Interlayer Excitons in MoSe2-WSe2 Heterostructures 4. **Alexey Kavokin, Westlake U., China:** Qubits Based on Split-Ring Condensates of Exciton-Polaritons 5. **Yurii E. Lozovik, Spectroscopy Inst., Troitsk, Russia:** Superfluidity and BEC in Novel 2D Materials 6. **Massimo Rontani, CNR-NANO, Modena, Italy:** Excitonic Insulator in Long-Range Interacting Systems 7. **Klaus Ziegler, U. Augsburg, Germany:** Topological Phases Created by Electron-Phonon Interaction	1. **W.Jaskólski, Copernicus U., Poland:** Forcing Single Layer Graphene to Behave Like a Gated Bilayer 2. **T.Kereselidze, TSU, Georgia:** Electronic and Optical Properties of Ellipsoidally Shaped Nanoparticles 3. **S.A.Moskalenko, Applied Physics Inst., Moldova:** 2D Magneto-Excitons with Linear Dispersion Law under the Influence of the Quantum Point Vortices 4. **Sh.M.Tsiklauri, CUNY, USA:** Trions in Transition Metal Dichalcogenide and Buckled Monolayers
Polaritonics and Nonlinear Optics with Quantum Materials	1. **Sven Höfling, U. Wuerzburg/U. St.Andrews, Germany/UK:** Valley Selective Condensation and Expansion of Exciton-Polaritons Based on MoSe2 Monolayer Crystals 2. **Jacob Khurgin, J.Hopkins U., USA:** Waveguiding and Second Order Nonlinearities in Transition Metal Dichalcogenides 3. **Mark Stockman, Georgia State U., USA:** Quantum Solids in Ultrafast Strong Laser Fields: Topological Nanophotonic Phenomena 4. **David W. Snoke, U. Pittsburgh, USA:** Polariton Condensates with Long Lifetime and Long-Distance Transport 5. **David Tománek, Michigan State U., USA:** Magic with 2D Semiconductors	1. **F.Benimetskiy, ITMO, Russia:** Strong Coupling of Excitons in Direct Bandgap 2D Semiconductor with Optical Bound States in the Continuum 2. **O.Berman, CUNY, USA:** Spin Hall Effect for Microcavity Polaritons in Transition Metal Dichalcogenides

B. POSTER PRESENTATIONS (presenter's last name alphabetical order)

- **B.Beradze, TSU, Georgia:** Magnetic Phase Diagram of a Spin-1/2 Antiferromagnetic Two-Leg Ladder in the Presence of Modulated along Legs Dzyaloshinskii-Moriya Interaction
- **A.M.Grudinina, MEPhI, Moscow, Russia:** Ground State of an Anisotropic 2D Exciton and Magneto-Exciton in Phosphorene Monolayer and Bilayer
- **L.Jibuti, TSU, Georgia:** Study of Resistive Switching Effect in the Si+W+ZrO2+HfO2+Mo+Al Nanostructure
- **V.A.Kuznetsov, Solid State Phys. Inst., Chernogolovka, Russia:** Excitonic Effects and Non-Trivial Spin Polarization at Filling Factor of 3/2
- **Z.Machavariani, TSU, Georgia:** Trions and Biexcitons in Core/Shell Nanowires
- **Jason D. Orlando, NCCU, USA:** Surface-Enhanced Raman Scattering Characteristics of Gold Nanoparticle-Decorated WS2 Nanosheets
- **M.V.Rakhlin, Ioffe Inst., St-Petersburg, Russia:** Efficient Single-Photon Sources of Red Light Based on a Waveguide Photonic Nanoantenna with an InAs/AlGaAs Quantum Dot
- **Giacomo Sesti, U. Modena, Italy:** Anomalous Screening in Narrow-Gap Carbon Nanotubes

POSTER PREPARATION INSTRUCTIONS: Poster Format – Portrait A0 841 mm × 1189 mm (33.1 in × 46.8 in); tapes/pins will be provided

Preface

The booklet contains the program and the abstracts of the International School and Workshop on Two-Dimensional Crystals and Photonics held at Ivane Javakhishvili Tbilisi State University, Tbilisi, Georgia.

The event is expected to gather internationally recognized leaders in the field, scientists and researchers, to present their talks about the most important latest developments in this new important research field. Topics will include but will not be limited to:

(1) 2D Plasmonics and Metasurfaces;
(2) Physics of Excitons in Low-Dimensional Semiconductors;
(3) Polaritonics and Nonlinear Optics with Quantum Materials.

The main objective of this School and Workshop is to get together the recognized leaders in the field to discuss the most critical technological advances, innovations, fundamental aspects and a broad range of applications, from chemistry and fabrication of nanomaterials to photonic and optoelectronic systems with new quantum materials of reduced dimensionality. The School and Workshop provides a unique platform for the leading experts to meet, share knowledge and establish collaborative ties in rapidly developing research fields such as Optoelectronics and Photonics, Quantum Materials, Metasurfaces and Ultrathin Films. Students and early career researchers attending the conference will have unique opportunities to interact with the prominent research leaders and experts in Physics of Low-Dimensional Structures and Photonics.

The 2DCP International School and Workshop will feature the state-of-the-art lectures by internationally recognized experts in the field, seminars by prominent mid-career researchers and poster sessions by workshop participants. The School and Workshop will facilitate existing research partnerships and will promote new scientific and academic collaborations. It will help establish and solidify mutually beneficial ties between international research groups actively working in the field, between young and experienced researchers.

International Program Committee

Table and Contents

Magic with 2D Semiconductors

David Tománek
Physics and Astronomy Dept., Michigan State University, East Lansing, MI 48824, USA
tomanek@pa.msu.edu

Like in a magic trick, atomically thin layers of specific materials can be mixed and stacked in a well-defined way. Due to the inter-layer interaction and charge transfer, the heterostructure may exhibit sometimes unexpected behavior. This occurs in the case of elemental boron, which is notorious for a large number of stable allotropes not only in 3D bulk, but also in 2D. We find that a previously unknown 2D ε–B allotrope converts stepwise to a stable honeycomb structure when doped with electrons, resembling a magic conversion of boron to carbon atoms that carry one more valence electron [1]. As seen in Fig. 1(b), sufficient extra charge to initiate this transition may be provided when 2D boron is brought into contact with the 2D electride Ca_2N. A different apparent example of magic involves the previously overlooked twist degree of freedom in 2D structures like bilayer graphene, which changes the Moiré pattern, as shown in the left panel of Fig. 1(c). Recent theoretical and experimental evidence suggests that the electronic structure near the Fermi level of twisted bilayer graphene (TBLG) depends extremely sensitively on the twist angle θ. Near the magic angle value $\theta_m \approx 1.08°$, a flat band emerges at E_F, separated from conduction and valence states by energy gaps. This unexpected behaviour likely provides valuable insight into electron correlation and superconductivity in 2D systems. Even though TBLG and related non-periodic structures can not be treated by standard band structure theory, their electronic structure can be interpreted quantitatively using a parameterized model [2] that can be simply extended to consider also other deformations including shear [3].

This study was partly supported by the NSF/AFOSR EFRI 2-DARE grant number #EFMA-1433459.

References

[1] Dan Liu and David Tománek, *Effect of Net Charge on the Relative Stability of 2D Boron Allotropes*, *Nano Lett.* **19**, 1359-1365 (2019).
[2] Xianqing Lin and David Tománek, *Minimum model for the electronic structure of twisted bilayer graphene and related structures*, *Phys. Rev. B.* **98**, 081410(R) (2018).
[3] Xianqing Lin, Dan Liu and David Tománek, *Shear instability in twisted bilayer graphene*, *Phys. Rev. B.* **98**, 195432 (2018).

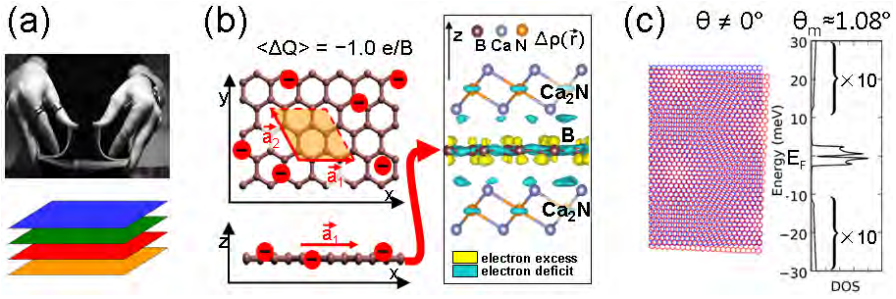

Figure 1: (a) Card magic illustrating the van der Waals assembly of 2D materials to a functional nanostructure. (b) Conversion of a 2D boron monolayer to a honeycomb lattice due to electron doping provided by a 2D electride. (c) Unusual changes in the electronic structure of twisted bilayer graphene near the magic twist angle $\theta_m \approx 1.08°$.

Valley selective condensation and expansion of exciton-polaritons based on $MoSe_2$ monolayer crystals

Christian Schneider[1,*], M. Waldherr[1], N. Lundt[1], M. Klaas[1], L. Dusanovski[1], S. Tongay[2], E. Ostrovskaya[3], A. Kavokin[4], S. Höfling[1,5]

[1] *Technische Physik and Wilhelm Conrad Röntgen-Center for Complex Material Systems, University Würzburg, Am Hubland, 97074 Würzburg, Germany*

[2] *School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, AZ 85287, USA*

[3] *ARC Centre of Excellence in Future Low-Energy Electronics Technologies and Nonlinear Physics Centre, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 2601, Australia*

[4] *WIAS, Shilongshan Road, Cloud Town, Hangzhou, China*

[5] *SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews, KY169SS, UK*

*Corresponding author: *christian.schneider@uni-wuerzburg.de*

Condensation of bosons into a macroscopic quantum state belongs to the most intriguing phenomena in nature, which became accessible in open-dissipative, exciton-based solid-state systems at elevated temperatures. Semiconducting monolayer crystals have emerged as a new platform for studies of strongly bound excitons and exciton-polaritons [1] in ultimately thin materials. We discuss the formation of a bosonic condensate driven by excitons hosted in an atomically thin layer of $MoSe_2$, strongly coupled to light in a solid-state resonator [2]. Polariton condensation manifests by a superlinear increase of emission intensity from the hybrid polaritons. The mode experiences a collapse of the emission linewidth, a core sign of temporal coherence. With increasing pump power, we observe a blueshift of our resonance which originates from particle interaction with free excitons in the uncondensed reservoir states. Importantly, we observe a significant spin-polarization in the injected polariton condensate, a clear sign for valley-selective condensation in our crystal.

In turn, high fidelity spin-selective, as well as valley-coherent injection of valley exciton-polaritons is demonstrated via resonant, non-linear spectroscopy. In contrast to previous experiments based on excitons in bare $MoSe_2$ monolayer crystals, valley polarization and coherence can be retained to a very high degree the MoSe2 polariton-system. As a consequence, valley selective polariton currents emergy in the expanding polariton cloud, which is a manifestation of the optical valley Hall effect in the hybrid light-matter system.

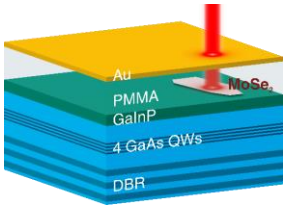

Figure 1: Hybrid Tamm-plasmon device with an embedded $MoSe_2$ monolayer. Collective strong light-matter coupling between the cavity mode and the excitonic resonances from the $MoSe_2$ and GaAs layers give rise to hybrid polariton modes. We observe the formation of an exciton-polariton condensate caused by amplified bosonic scattering into the ground state.

References

[1] C. Schneider et al. Nature Communications **9**, 2695 (2018).

[2] M. Waldherr et al. Nature Communications **9**, 3286 (2018).

Excitonic insulator in long-range interacting systems

Massimo Rontani [1,*]
[1]*CNR-NANO, Via Campi 213a, 41125 Modena, Italy*
*Corresponding author: *massimo.rontani@nano.cnr.it*

Fifty years ago a few outstanding physicists, including Leonid Keldysh and Walter Kohn, put forward a heretic paradigm of a strongly correlated insulator: If a narrow-gap semiconductor (or a semimetal with slightly overlapping conduction and valence bands) failed to fully screen its intrinsic charge carriers, then excitons---electron-hole pairs bound together by Coulomb attraction---would spontaneously form. This would destabilize the ground state, leading to a reconstructed 'excitonic insulator' that would exhibit a distinctive broken symmetry, inherited by the exciton character, as well as peculiar collective modes of purely electronic origin. Intriguingly, the excitonic insulator, which shares similarities with the Bardeen-Cooper-Schrieffer superconducting ground state, could display unusual macroscopic quantum coherence effects. So far, the observation of this phase has been elusive. The crux of the matter is the trade-off between competing effects in the semiconductor: as the size of the energy gap decreases, favouring spontaneous exciton generation, the screening of the electron-hole interaction increases, suppressing the exciton binding energy.

Very recently, novel low-dimensional systems seem to renew the promise of the excitonic insulator, as they combine optimal band structures, poor screening, truly long-ranged interactions, and giant excitonic effects. In this talk, after reviewing key concepts and breakthroughs, I will discuss our theoretical results concerning narrow-gap carbon nanotubes [1] and layered transition metal dichalcogenides, based on the combination of first-principles and model approaches.

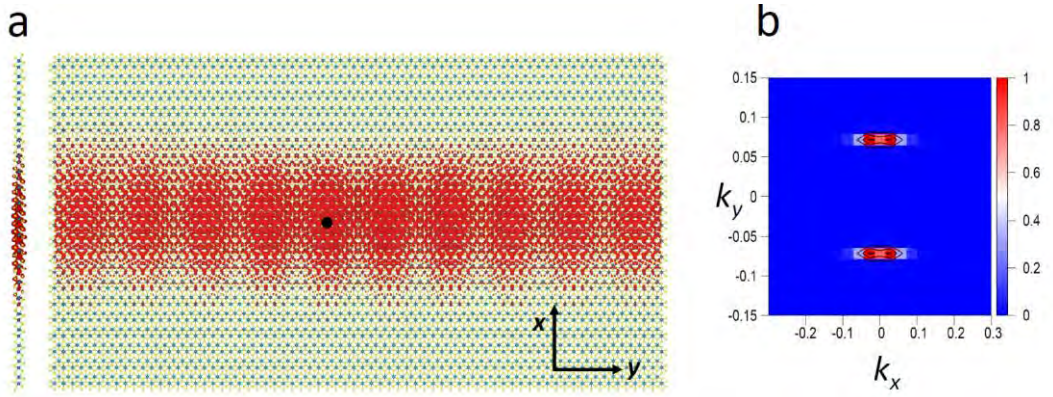

Figure 1: First-principles wave function of the lowest-energy exciton of *T'*-MoS_2, a 2d topological insulator. The binding energy of this exciton is larger than the gap, hence the system is unstable against the spontaneous generation of excitons. **a,** Exciton wave function square modulus, as obtained from Bethe-Salpeter equation. The contour plot (red colour) is the probability density to locate the bound electron once the hole position is fixed (black dot). The figure contains 21 and 69 unit cells in the *x* and *y* direction, respectively. Note the delocalization in real space along the *y* direction of Mo zig-zag chains. **b,** Exciton wave function square modulus in **k** space region around the Λ points. After D. Varsano, M. Palummo, E. Molinari, M. Rontani (2019), unpublished.

This work is done together with D. Varsano, E. Molinari, S. Ataei, G. Sesti, M. Palummo, D. Sangalli, S. Sorella, S. Corni, M. Barborini. I acknowledge support from projects EU H2020-INFRAEDI-2018 No. 824143 "MaX" and MIUR-PRIN2017 No. 2017BZPKSZ "EXC-INS".

References

[1] D. Varsano *et al*., Nature Communications **8,** 1461 (2017).

Controlling Infrared Light with Nanoscale Precision Using 2D Material Polaritons

Joshua D. Caldwell,[1,*]
[1]*Dept. Mechanical Engineering, 2400 Highland Ave, Nashville, TN 37205 USA*
*Corresponding author: *josh.caldwell@vanderbilt.edu*

The current state-of-the-art in materials used for IR optical components offers significant material limitations. This is exacerbated by the long free-space wavelengths in this spectral region. Through the use of polaritons, one can surpass the diffraction limit and thus these limitations can be circumvented. However, the predominant types of polaritons employed, the surface plasmon (SPP) and surface phonon polaritons (SPhP) are typically realized within epitaxial semiconductors and dielectrics in the IR, restricting the design space due to lattice match requirements. In contrast, two-dimensional materials offer a broad suite of alternative semiconductor, conductor and dielectric species with atomic-scale thickness control and "Lego-like" stacking enabling arbitrary heterostructure and superlattice designs. Further, the natural crystal anisotropy resulting from the strong covalent in-plane and weak van der Waals out-of-plane bonds gives rise to extreme birefringence and in many cases hyperbolicity, offering new pathways for on-chip photonics and compact optical components. In 2014, it was demonstrated that hexagonal boron nitride (hBN) was a natural hyperbolic material,[1,2] serving as the basis for applications such as hyperlensing.[3,4] More recently, it was demonstrated that MoO_3 offers strong out-of-plane and *in-plane* hyperbolicity.[5]This provides the potential basis for deeply sub-diffractional waveplates, polarizers and polarized thermal emitters.[6] This talk will address the potential for leveraging such large crystal anisotropy for realizing reconfigurable planar metasurfaces,[7] flat and compact IR components and actively tunable and modulated IR optics.

References

[1] Caldwell, JD *et al.*, Nat Comm **5**, 5221 (2014).
[2] Dai, S *et al.*, Science **343**, 1125-1129 (2014).
[3] Dai, S *et al.*, Nat Comm **6**, 6963 (2015).
[4] Li, P *et al.*, Nat Comm **6**, 7507 (2015).
[5] Ma, W *et al.*, Nature **562**, 557-562 (2018).
[6] Folland, TG *et al.*, Nature **562**, 499-501 (2018).
[7] Folland, TG *et al.*, Nat Comm **9**, 4371 (2018).

Superfluidity and BEC in Novel 2D materials

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New effects in systems of quantum dipolar excitons are discussed, such as anisotropic superfluidity in external fields, strong correlations, crystallization, the supersolid phase etc.(see [1,2] and cited refs). Roton instability effects typical of strongly correlated Bose systems but also manifesting themselves in weakly interacting systems of titled dipoles are analyzed. Among the interesting physical realizations of the systems under consideration are dipole excitons in single or coupled quantum wells and in van der Waals heterostructures of new 2D materials, such as transition metal dichalcogenides (TMDCs).

We consider a bilayer system of two-dimensional Bose-Einstein-condensed dipolar dark excitons (upper layer) and bright ones (bottom layer) [3]. We demonstrate that the interlayer interaction leads to a mixing between excitations from different layers. This mixing leads to the appearance of a second spectral branch in the spectrum of bright condensate. The excitation spectrum of the condensate of dark dipolar excitons then becomes optically accessible during luminescence spectra measurements of the bright condensate, which allow probing its kinetic properties. This approach is relevant for experimental setups, where detection via conventional techniques remains challenging, in particular, the suggested method is useful for studying dark dipolar excitons in transition metal dichalcogenide (TMDC) monolayers.

We propose a method to increase the lifetime of two-dimensional direct excitons and show the possibility to observe their macroscopically coherent state at temperatures much higher than that of indirect exciton condensation [4]. For a single GaAs quantum well embedded in photonic layered heterostructures with subwavelength period, we predict the exciton radiative decay to be strongly suppressed. Quantum hydrodynamics joined with the Bogoliubov approach are used to study the Berezinskii-Kosterlitz-Thouless crossover in a finite exciton system with intermediate densities. Below the estimated critical temperatures, drastic growth of the correlation length is shown to be accompanied by a manyfold increase of the photoluminescence intensity.

Controlling of 2D excitons in external fields will be discussed.

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Topological phases created by electron-phonon interaction

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A 2D electron-hole gas with a Dirac node in the spectrum is coupled to in-plane phonons. At sufficiently strong interaction the system undergoes a second-order phase transition, in which the quasiparticles become spontaneously massive. The new phase has topological properties, characterized by nonzero Chern numbers. Calculations of the transport properties via the Kubo formalism indicate a quantized Hall conductivity. This is associated with a Chern-Simons field theory, which allows us to study the response to different external fields and to analyze the topological phase transition.

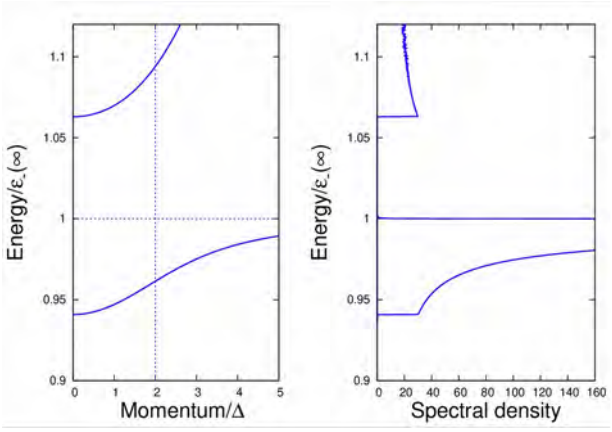

Figure 1: Two branches of the ``polariphon'' spectrum with an avoided crossing [1]

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Unexpected Magnetism in Semiconducting Transition Metal Dichalcogenides

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Transition metal dichalcogenides (TMDs) are interesting for understanding the fundamental physics of two-dimensional (2D) materials as well as for applications to many emerging technologies, including spin electronics. We report the discovery of long-range magnetic order below T_M = 40 and 100 K in bulk semiconducting TMDs 2H-$MoTe_2$ and 2H-$MoSe_2$, respectively [1]. The presence of long-range magnetism is remarkable because these semiconductors do not contain magnetic ions. Density functional theory (DFT) calculations show that this magnetism is promoted by the presence of defects in the crystal. The scanning tunneling microscopy (STM) measurements show that the majority of defects in these materials are metal vacancies and chalcogen-metal antisites, which are randomly distributed in the lattice at the subpercent level.

Establishing long-range magnetic order with the observed low density of antisite defects would necessarily involve electronic coupling to the semiconductor valence electrons. The presence of such spin-polarized itinerant electrons implies that these materials are dilute magnetic semiconductors (DMSs) without need to dope with magnetic ions. Further, we found that the magnetic order stabilized in 2H-$MoTe_2$ and 2H-$MoSe_2$ is highly sensitive to hydrostatic pressure. These observations establish 2H-$MoTe_2$ and 2H-$MoSe_2$ as a new class of magnetic semiconductors and open a path to studying the interplay of 2D physics and magnetism in these interesting semiconductors.

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Waveguiding and Second Order Nonlinearities in Transition Metal Dichalcogenides

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In the first part of the presentation I will consider the possibility of light guiding by a single monolayer of 2D material. Two-dimensional (2D) monolayer-thick materials with a direct bandgap, such as MoS2, WSe2, and other transition metal dichalcogenides (TMDCs), are being actively explored for future nanophotonic applications in the visible and UV ranges. In this presentation I will show that a monolayer of TMDCs is capable of supporting a guided optical mode below the exciton resonance—a 2D exciton–polariton. I evaluate the characteristics of these guided modes and conditions required for their existence, including derivations of mode dispersion relations, mode confinements, and propagation lengths. The visible or near-IR mode is confined to within roughly a micrometer of the monolayer and has a propagation length exceeding 100 μm. This light guiding ability in the visible and IR ranges makes TMDC monolayers a versatile and potentially attractive platform for future optoelectronic devices.
The second part of the talk will be dedicated to the second order nonlinear properties of TMDC's – from a single monolayer to a few layers. Controlling nonlinear light−matter interaction is important from a fundamental science point of view as well as a basis for future optoelectronic devices. Recent advances in two-dimensional crystals have created opportunities to manipulate nonlinear processes electrically. Here I will present the result on a strong second harmonic generation (SHG) in a 2D WSe2 bilayer crystal caused by a back gate field. This unusual process takes place only when the gate polarity causes charge accumulation rather than depletion. Analysis based on a bond−charge model traces the origin of SHG to the nonuniform field distribution within a single monolayer, caused by the accumulated sub-monolayer screening charge in the tungsten plane. I name this phenomenon charge-induced SHG (CHISHG), which is fundamentally different from the field- or current-induced SHG. These findings provide a potentially valuable technique for understanding and noninvasive probing of charge and current distributions in future low dimensional electronic devices.
I will conclude with examining nonlinearities in the combined plasmonic-TMDS structures.

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Cavity and magnetic field effects on interlayer excitons in MoSe2-WSe2 heterostructures

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Optical properties of interlayer excitons in lattice-incommensurate or twisted MoSe2-WSe2 heterobilayers are predicted to exhibit substantial modifications by moiré superlattice potentials [1]. In contrast, MoSe2-WSe2 heterostructures grown by chemical vapor deposition are free of moiré effects due to lattice-mismatch relaxation and inherent orientational alignment [2]. Using such moiré-free heterostructures, we performed cryogenic studies of interlayer excitons subjected to cavity and magnetic field effects. Our cavity-assisted experiments demonstrate Purcell enhancement for interlayer exciton photoluminescence, and quantify the respective light-matter coupling strength [3]. In complementary magnetoluminescence experiments, we study valley polarization dynamics of interlayer excitons with indications for accumulation of valley polarization in valley-dark exciton reservoirs and polarization transfer to resident charge carriers present due to residual doping.

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Excitonic complexes in semiconductor and graphene quantum dots

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We discuss here excitonic complexes in semiconductor and graphene quantum dots. After general introduction to excitons as many-body excitations we will describe our approach to optical properties of million atom nanostructures, QNANO. Using atomistic tight binding description of single particle states, efficient computation of Coulomb matrix elements and configuration interaction approach we describe excitons, bi-excitons, multi-excitons and trions in optical processes of graphene [1-4] quantum dots, single 2D layer of transition metal dichalcogenites (TMDCs)[5-7], semiconductor self-assembled quantum dots [8-10] and semiconductor colloidal nanocrystals[10-12]. We focus on the exciton spectrum, exciton fine structure and bi-exciton-exciton cascade in self-assembled InAs quantum dots in InP nanowires [9], exciton-bi-exciton Auger mixing in CdSe nanocrystals[10] as well as topological excitons and robust trions [7] in TMDCs. We will contrast excitons in semiconductor self-assembled quantum dots with graphene and nanocrystals. We will show that there exists a degeneracy of the top of the valence band both in semiconductor and graphene nanocrystals. This leads to a peculiar exciton spectrum in graphene analogous to the spectrum of the p-shell of self-assembled quantum dots. The degeneracy, e-e interactions and strong Auger mixing prevent applications of nanocrystals as lasers and diodes. We describe a selective facet epitaxy as means of reengineering of energy spectrum of a 2D nanocrystal solid enabling lasing [12].

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Plasmonics in two-dimensional crystals[1,2,*]

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Two-dimensional materials have been recently shown to host robust polaritonic modes, ranging from plasmons in highly doped graphene to excitions in transition metal dichalcogenides. The electromagnetic behavior of these modes can be well understood in terms of an effective surface conductivity, in which we can capture their strong dependence on temperature and external static electric and magnetic fields. Recent advances have also been produced in the synthesis of thin noble-metal films, which open new possibilities for exploring entirely new regimes of nanometallic plasmonics. In this talk, I will overview the general characteristics of the optical response of these materials, which we can understand in terms of simple theoretical descriptions. We will also cover more sophisticated descriptions, aiming at exploring genuinely quantum-mechanical effects. We will further overview recent advances in ultrafast optical response and nonlinear optics, as well as the potential application of these materials for light modulation, quantum-optics, and optical sensing.

Quantum Solids in Ultrafast Strong Laser Fields: Topological Nanophotonic Phenomena

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We present the latest theoretical predictions and recent experiments on behavior of novel quantum materials – two dimensional solids, topological insulators, and Weyl semimetals – in ultrafast, strong, chiral laser fields. This behavior is determined by the topology of the solids' reciprocal space. It opens new avenues in quantum physics and quantum information.

A strong optical field, ~0.1-1 V/Å, changes solids on the attosecond time scale, i.e., within an optical cycle. Such fields drive ampere-scale currents in dielectrics and adiabatically controls their properties, including optical absorption and reflection, extreme UV absorption, and generation of high harmonics in a non-perturbative manner [1-5].

We concentrate on ultrafast phenomena defined by nontrivial topological properties of solids in the reciprocal space, which are described by non-zero Berry (topological) curvature and Berry flux, which to a significant degree define their behavior in strong optical fields. In particular, these are graphene [6,7], silicene [8], and surfaces of topological insulators (TI's) (semimetals) [9], monolayer transition metal dichalcogenides (TMDC's) [10], black phosphorus and phosphorene (direct bandgap semiconductors), and hexagonal boron nitride (h-BN) (dielectric).

For two-dimensional semiconductors such a TMDC's, we predict a new attosecond phenomenon in a strong chiral optical fields – a topological resonance [11]. This manifests itself in the establishment of a strong valley polarization during just a single optical cycle, i.e., in the fundamentally fastest way possible. It structures the reciprocal space into topologically distinct areas. This phenomenon is promising for ultrafast recording of both classical bits and cubits for quantum information processing.

Another distinct class of two-dimensional systems in a strong pulse field that we consider are surfaces of TI's. These are crystals characterized a non-zero topological invariant Z2=1 where bulk is semiconducting but surfaces are Dirac semimetals. In the surface reciprocal space, they contain a single Dirac point with a Berry phase of $\pm\pi$ at the Γ-point. Subjected to circularly-polarized ultrashort strong pulses they exhibit chiral textures in the reciprocal space and topologically-protected currents [9].

Finally, we present our latest results on Weyl semimetals in ultrafast strong chiral fields. Such fields induce topological resonances and ultrafast bulk currents on femtosecond time scales.

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Polariton Condensates with Long Lifetime and Long-Distance Transport

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In the past few years, microcavity structures have become available with long polariton lifetime (~ 200 ps at resonance) and long-distance transport (hundreds of microns). This has allowed numerous new observations including Bose-Einstein condensation of polaritons in a trap in equilibrium, quantized circulation in a ring trap, and observation of the Thomas-Fermi regime of a condensate at high density. Recently, we have performed time-resolved imaging and spectroscopy of a polariton condensate in a one-dimensional ring geometry, starting from a highly nonequilibrium state and evolving all the way to an equilibrium condensate. Near equilibrium, the condensate undergoes damped oscillations at the natural frequency of the trap. This talk will review the general theory and design of microcavity polariton structures, discuss the implications of recent experiments for the elusive value of the polariton-polariton interaction constant, which is an important parameter for theories of nonlinear optics with polariton systems, and will also review how the Gross-Pitaevskii equation must be modified to model the polariton condensate with damping.

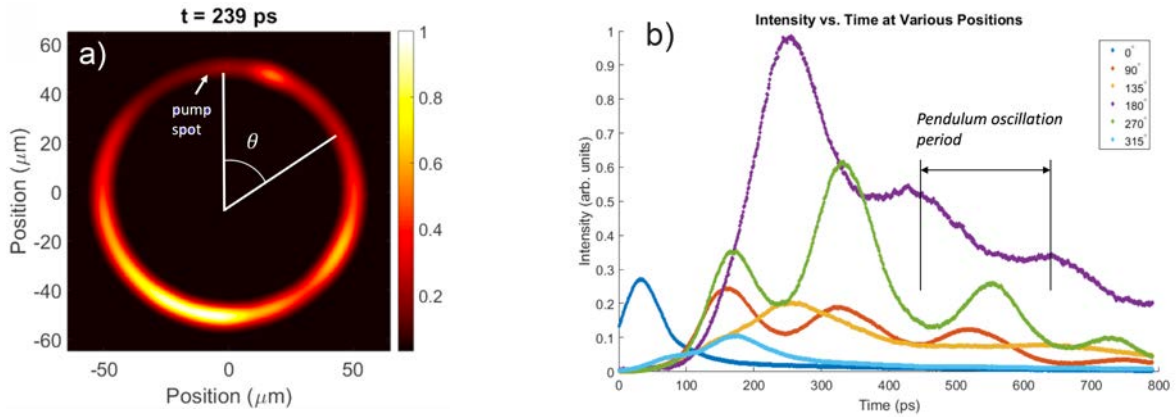

Figure 1. a) Snap shot from a movie (available at [https://tinyurl.com/y97x7yap)](https://tinyurl.com/y97x7yap) of the polariton motion in a ring. b) The intensity as a function of time at various points on the ring, for a typical experiment.

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Trapping excitons in monolayers and heterostructures of atomically-thin semiconductors

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Quantum light sources in solid-state systems are of major interest as a basic ingredient for integrated quantum photonic technologies. In particular, the ability to site-selectively *create* quantum emitters and *position* them relative to nanophotonic structures (e.g. cavities or waveguides) would be a major step on the road towards integrated technologies. For quantum emitters formed in atomically thin 2D materials, several approaches have been explored to trap excitons including using local-strain, environmental dielectric contrast and the site-selective generation of luminescent point defects. In this talk we will explore each of these approaches and present recent results from our lab. We will begin by exploring the site-selective generation of quantum emitters in hBN encapsulated MoS_2 using **local He-ion irradiation** [1,2]. Here, upon dosing a ~100x100nm region of the hBN encapsulated MoS_2 with He-ions we observe spectrally narrow emission lines within a narrow energy window ~190±10meV below the neutral 2D exciton. Ab-initio calculations indicate that these emission lines stem from the recombination of highly localized electron-hole complexes at Mo-vacancies created by the He-ion beam. In a second experiment, we trap a tunable number of dipolar interlayer excitons ($N_{IX} \sim 1-4$) within a nanoscale confinement potential induced by placing a $MoSe_2$-WSe_2 hetero-bilayer onto an array of SiO_2 nanopillars [3,4]. We control the mean occupation of the IX trap via the optical excitation level and observe discrete sharp-line emission from different configurations of localized IXs, the intensity of which exhibit characteristic linear, quadratic, cubic and quartic power dependencies [5]. These observations allow us to identify these features as single and multiple localized IX and facilitate the direct measurement of the hierarchy of dipolar and exchange inter- actions. The interlayer bi exciton ($N_{IX} = 2$) is found to be an emission doublet that is blue-shifted from the single exciton by $\Delta E = (8.4 \pm 0.6)$ meV and split by $2J = 1.2 \pm 0.5$meV. These values are shown to be mutually consistent with numerical modelling of dipolar excitons moving in a harmonic trapping potential having a confinement length scale in the range $\ell \sim 3-4$ nm [6, 7]. Our results contribute to the understanding of interactions between IX in TMD hetero- bilayers at the discrete limit of only a few excitations and represent a key step towards studying quantum correlations between IXs in TMD hetero-bilayers.

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Two-dimensional magnetoexcitons with linear dispersion law under the influence of the quantum point vortices

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1. The exchange *e-h* Coulomb scattering takes place with the annihilation and the creation of the *e-h* pairs with the resultant electronic charges equal to zero. They have dipole-dipole interaction, when the interband dipole moments ρ_{c-v} are different from zero. It happens when the crystals have the dipole active optical quantum transitions. We have considered the semiconductor layers of the type *GaAs* with *s*-type conductions band and *p*-type valence band with magnetoexcitons formed by electrons with spin projections $s_z^e = \pm 1/2$ and by heavy holes with full angular momentum projections $j_z^h = \pm 3/2.$ The Lorentz force in the Landau gauge description determines the positions of the Landau quantization oscillations of the electrons and holes and their distances in the frame of the magnetoexcitons. Their relative and center of mass motions are interconnected. In difference on the direct Coulomb *e-h* interaction, which gives rise to the quadratic dispersion law $\hbar^2 k^2/2M(B)$ with magnetic mass $M(B)$ depending on the magnetic field strength B, the exchange *e-h* Coulomb interaction gives rise to linear dispersion law known as Dirac cone $\hbar \mathrm{v}_\mathrm{g} k$ with group velocity v_g depending on the interband dipole moment in the way: $\mathrm{v}_\mathrm{g} \approx \left|\rho_{c-v}/l_0\right|^2 \approx B,$ where l_0 is the magnetic length.

2. The thermodynamic properties of the ideal 2D Bose gas with linear dispersion law were discussed in the Ref [1]. The critical temperature of the Bose-Einstein condensation (BEC) of the 2D magnetoexcitons is different from zero even at the infinite homogeneous surface area and following [1] is proportional to the group velocity: $T_c \sim \mathrm{v}_\mathrm{g} \sim B.$ In the case of the magnetoexcitons it increases with the increasing magnetic field strength *B*.

3. It was shown that the Chern-Simons (*C-S*) gauge field created by the quantum point vortices in the conditions of the fractional quantum Hall effects (*FQHEs*) leads to the formation of the composite electrons and holes with equal integer numbers of the attached to each particle quantum point vortices. The coherent superposition of the velocities of these vortices leads to the formation of the *C-S* vector potential, which depends on the difference between the density operators $\hat{\rho}_e$ of the electrons and $\hat{\rho}_h$ of the holes. The *C-S* vector potential generates the effective magnetic field acting on the particles in addition to the external magnetic field. In the mean field approximation, when the average densities of electrons and of the holes coincide the effective *C-S* magnetic and electric fields vanish and the Landau quantization of the composite particles with the bare electron and hole effective masses take place only under the influence of the external magnetic field [3].

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Spin Hall effect for microcavity polaritons in TMDCs

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We predict the spin Hall effect for polaritons (SHEP) in a transition metal dichalcogenides (TMDC) monolayer embedded in a microcavity [1]. As shown in Figure 1, two Bragg mirrors placed opposite each other at the antinodes of the confined photonic mode form a microcavity, and a TMDC layer is embedded parallel to the Bragg mirrors within the cavity. The cloud of *A* and *B* polaritons is formed due to the coupling of *A* and *B* excitons created in a TMDC monolayer and microcavity photons. It is demonstrated that two counterpropagating laser beams incident on a TMDC monolayer can split normal and superfluid polariton flows due to the generation the effective spin-dependent gauge vector and scalar potentials. Two coordinate-dependent, counterpropagating and overlapping laser beams in the plane of the TMDC layer interact with a cloud of polaritons. These laser beams produce the spin-dependent gauge magnetic and electric fields due to strong spin-orbit coupling for electrons and holes in TMDC. We show that the polariton flows in the same valley are splitting: the superfluid components of the *A* and *B* polariton flows propagate in opposite directions along the counterpropagating beams, while the normal components of the *A* and *B* polaritons flows slightly diverge and propagate almost perpendicularly to the superfluid flows. We obtained the components of polariton conductivity tensor for polaritons without Bose-Einstein condensation (BEC) and in the presence of BEC and superfluidity. The possible experimental observation of the SHE for microcavity polaritons, which provides the signature of the superfluidity of microcavity polaritons, is discussed.

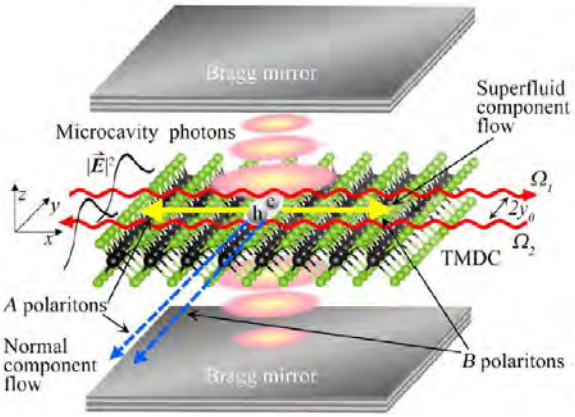

Figure 1: Schematic representation of the SHEP in a TMDC monolayer. The solid and dashed lines with arrows show the directions of deflected superfluid and normal flows of A and B polaritons, correspondingly. Two counterpropagating laser beams are shown by waved lines.

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Trions in transition metal dichalcogenide and buckled monolayers

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The positive and negative trions in two-dimensional (2D) transition metal dichalcogenides (TMD) namely MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2 and in buckled monolayers of silicene, germanene, and stanine, which we referred as Xenes, are studied in the framework of a nonrelativistic potential model by employing method of hyperspherical harmonics (HH).
The interaction potential between charge carriers is assumed to be of the Rytova-Keldysh (RK) potential [1], which takes into account of the strong screening due to the reduction of dimensionality. At a larger inter-particle separation, this interaction has the three-dimensional Coulomb tail, while at very small distances it becomes a logarithmic potential of a point charge in two dimensions. In the framework of the effective-mass approximation, we solve the three-body Schrödinger equations with the RK potential by expanding the wave functions of a trion in terms of the antisymmetrized HH [2]. Theoretical analysis is performed to provide a symmetry classification of the trion states in TMD, with an additional quantum number - the valley index. In the diagonal approximation, we present the analytical solution for the binding energy and wave function for two asymptotic cases: for a very larger electron-hole separation and for very small distances between charge carriers.
The binding energy of the trion depends significantly strongly on the dielectric environment. Our calculations performed for different sets of electron and hole masses show that binding energy for a negatively charged (T^-) is always less than for the positively charged (T^+) trion [3]. For tungsten diselenide monolayer -WSe_2 the T^+ trion has a smaller binding energy as compared to T^-. Results of our calculations are compared with variational calculations and studies by means of density functional theory, path integral Monte Carlo method, the diffusion Monte Carlo approach and stochastic variational method. The comparison shows that our calculations for the binding energies are consistent with previous computational studies with the RK potential and are in reasonable agreement with experimental measurements of the trion binding energies in TMD.

For trions in Xenes monolayers it is demonstrated that an external electric field can be used to tune the eigenenergies of the trions by changing the effective mass of charge carriers. In this case the three-body Schrödinger equation with field-dependent electron and hole effective masses [4] is also solved by using the RK potential.

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Strong coupling of excitons in direct bandgap 2D semiconductor with optical bound states in the continuum

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Over the last decade, the field of two-dimensional layered materials has seen rapid progress. Monolayers of transition-metal dichalcogenides (TMDCs) such as WS_2, MoS_2, WSe_2 and $MoSe_2$ have attracted strong interest as they exhibit direct bandgaps [1] and can be used as basic elements in compact photonics and optoelectronics devices. Furthermore, the ability to control light-matter interaction via exciton-photon coupling in hybrid systems consisting of such two-dimensional crystals and photonic structures enables a broad range of applications such as optoelectronic and MEMS devices, sensors, etc.

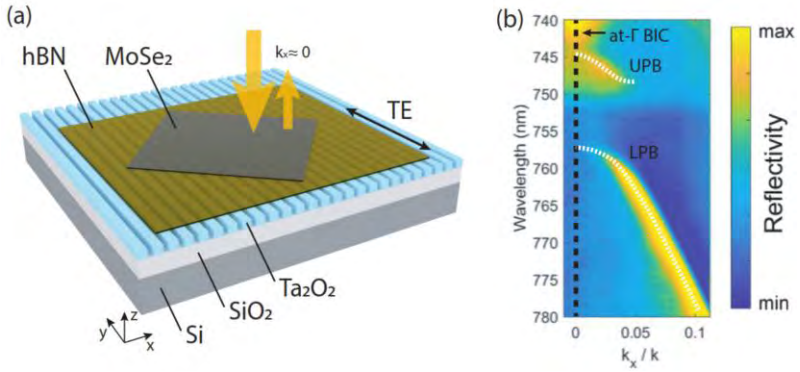

Figure 1: (a) Schematic of the Ta_2O_5 subwavelength grating with a $MoSe_2$/hBN heterostructure placed on top. (d) Angle-resolved reflectance spectra of the PCs-TMDC structure, showing splitting of the mode into upper and lower polariton branches (UPB and LPB).

Here we experimentally demonstrated exciton-photon coupling in a $MoSe_2$/hBN heterostructure interfaced with a Ta_2O_5 subwavelength grating structure (Fig.1(a)) supporting high-Q optical bound state in the continuum [2]. The resulting exciton-polaritons are probed by angle-resolved reflectivity and photoluminescence at 10 K (Fig.1(b)). We systematically investigate the temperature and polarization dependence of the polariton dispersion and associated Rabi splittings in the hybrid nanophotonic/TMDC structures through fitting the experimental data with finite-element numerical simulations. We further discuss the role of high-Q bound states in the continuum (BIC) modes supported by sub-wavelength gratings in the formation of strongly-coupled exciton-polaritons. Our results suggest a new platform for future TMDC-based polaritonic devices.

This work was supported by the Ministry of Education and Science of Russian Federation (project 14.Y26.31.0015).

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Plasmonic nanoparticle reflectors for hBN planar microcavities

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Combining plasmonic metals with 2D-materials such as transition metal dichalcogenides (TMDs) enables room temperature extreme nano-optics. Here we embed exfoliated hBN crystals in Au forming uniform planar half-microcavities and depositing Au nanoparticles on top form NP-on-microcavity (NPoMC) structures. These support new microcavity nano-resonator modes which can only be excited for TM polarization, and are extremely sensitive to the local environment.

Applications for ultralow energy optical switching motivate exploring resonator enhancement of their coupling. Fabricated van der Waals (vdW) heterostructure devices typically use hBN layers as an ideal dielectric substrate, and incorporation into optical resonators is thus of key interest. Utilizing plasmonic metals introduces rich nano-optics such as strong coupling to TMDs in WSe_2 [1], and enhanced emission [2], hence our study here of the Au/hBN system. Despite its simplicity, we find plasmonic scattering processes from Au nanoparticles on sub-micron thick hBN crystals are non-trivial, resulting in coupled microcavity-nanoparticle modes. We show that plasmonic nanoparticles can themselves form one mirror of a microcavity, producing a polarisation-dependent localised resonance. Admixing dipolar plasmonic scattering with Fabry-Perot interference produces modes surprisingly sensitive to scattering phase and incident angle.

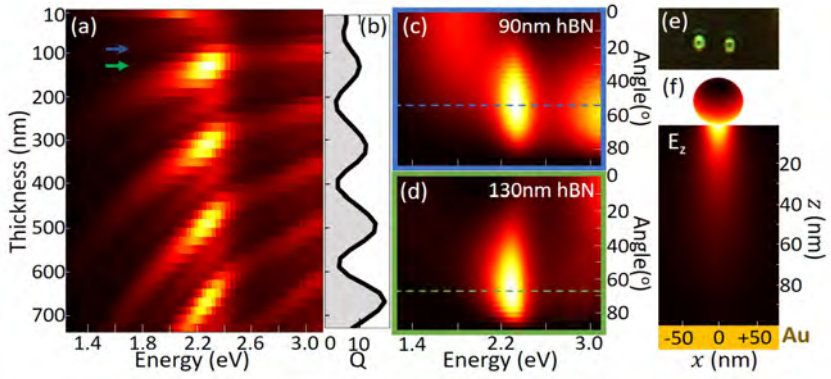

FIG.1 (a) Thickness dependence of TM scattering of nano-resonator modes, and (b) Q-factors. (c,d) Angle-dependent scattering at $\boldsymbol{L}$=90,130nm. (e) Scattering images at 100x magnification. (f) Scattered electric field for nano-resonator mode with $\boldsymbol{L}$=110nm, $\boldsymbol{\theta_i}$=58°.

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Forcing single layer graphene to behave like a gated bilayer

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It is demonstrated that single layer graphene can exhibit the electronic structure and properties of a gated bilayer, when it is properly attached to bilayer graphene. Here it is shown how to induce the energy gap, characteristic for gated bilayer, in the single layer graphene. Most importantly, we report on the appearance of topologically protected gapless state localized in a single graphene layer, when the bilayer exhibits the change in the stacking order. Therefore, the one-dimensional current in the topological state can flow in a single layer graphene, and this finding suggests a new exploitation of graphene in nanoelectronics.

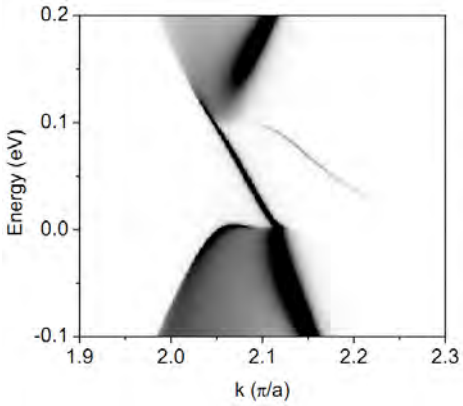

Figure 1: Local density of states calculated along the zigzag direction in the single layer graphene (SLG) properly attached to gated bilayer. Energy gap and topologically protected state are induced in the SLG.

Strongly correlated collective excitations in quasi-2D nanostructures of metals and semiconductors

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I will briefly review the latest experiments [1-7] and then enlarge on our theoretical efforts to develop the physical understanding of the properties of quasi-2D semiconductor and metallic nanostructures, efforts that have uncovered their intriguing optical attributes lending themselves to new attractive device applications. For instance, we show that the binding energies of the charged and neutral exciton complexes (trion and biexciton) formed by indirect excitons in layered quasi-2D semiconductors can be significant — up to a few tens of meV — for interlayer distances ~3–5 Å typical of transition metal dichalcogenide heterostructures [8]. This is now confirmed experimentally [7]. Exciton complexes in semiconductor coupled quantum wells and quasimonolayer van der Waals bound transition metal dichalcogenide systems are of interest for nonlinear optics and spinoptronics applications [5- 9]. We also develop a theory of the intra-intermolecular exciton intermixing and polarization dynamics for quasi-2D crystalline semi-conductors of organic molecules with two isolated low-lying Frenkel exciton states such as transition metal phthalocyanines [2,3]. The third-order nonlinear polarization response function we derive exhibits dynamical reorientation of the exciton transition dipole polarization (initially excited in the molecular plane) towards the axis of the molecular chain [3]. Such a dynamical reorientation pinpoints the preferential direction of the charge separation process for electron-hole pairs excited in these structures. Our results can be used for the proper interpretation of the optical properties of crystalline transition metal phthalocyanines — next generation organic semi-conductor materials for advanced optoelectronics. Last but not least, we study theoretically confinement related effects in the optical response of finite-thickness plasmonic films in the trans-dimensional regime [10-12] (between 3D and 2D [13-15]). We show that, while being constant for relatively thick films, the plasma frequency acquires spatial dispersion typical of 2D materials, gradually shifting to the red with the film thickness reduction. This explains experiments done on TiN films of controlled variable thickness [4], offering ways to tune the spatial dispersion and so the magneto-optical properties of plasmonic films and metasurfaces — not only by changing their composition but also by varying their thickness, aspect ratio, substrate and superstrate materials.

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Electronic and Optical Properties of Ellipsoidally Shaped Nanoparticles

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The physical properties of crystalline semiconductor structures of various shapes and nanometre size attract increasing interest. This interest is conditioned by the strong interdependence between the electronic, optical and mechanical properties of a nanoparticle object and its geometrical parameters.

Experiments indicate that small nanoparticles have a nearly spherical shape, whereas large nanoparticles have an ellipsoidal shape. At the growth of a nanoparticle with various methods, the electronic and optical properties vary continuously with its size and shape. An advantage of nanoparticles of ellipsoidal shape with respect to spherical quantum dots arises from the additional geometrical characteristics related to shape-anisotropy parameter β ($\beta = c/a$ in which c and a are prolate ellipsoidal semi-axes). That effect makes possible the tuning of the electronic and optical properties of objects of nanometre size. The tuneable control of characteristics of the nanometre objects through size and shape opens exciting possibilities for the engineering of new functional materials with a wide prospective application.

The analytical calculation of the energy spectrum and appropriate wave functions, for nanoparticles of an ellipsoidal shape, is a complicated task even in the one-particle approximation. The problem can be solved analytically using the small parameter appearing in the following two limiting cases: for the nanoparticles of a nearly rounded shape ($c \simeq a$) [1], and for the nanoparticles of strongly prolate ellipsoidal shape ($c \gg a$) [2]. For a charged particle trapped in a potential well of an ellipsoidal shape with arbitrary c and a, the problem was solved numerically [3]. Comparison shows that, in the regions of their validity, the energy levels obtained analytically are in good agreement with the numerical results.

The behavior of optical spectra of an electron (or hole) confined within a potential well of ellipsoidal shape is investigated as a function of shape-anisotropy parameter β. The optical transition-matrix elements are calculated in the dipole approximation using perturbation theory and with a direct diagonalization of the appropriate Hamiltonian. The matrix elements involving the ground and first excited states are monotonic functions of β, whereas matrix elements involving the highly excited states have zeros and extrema that are reflected in the behaviour of the corresponding transition probabilities [4]. Moreover, some matrix elements involving the excited states have discontinuity; the origin of this discontinuity is revealed. The profiles of a spectral line emitted or absorbed by an ensemble of ellipsoidally shaped nanoparticles with a Gaussian distribution of size are calculated and discussed [5].

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Surface-enhanced Raman Scattering Characteristics of Gold Nanoparticle-Decorated WS_2 Nanosheets

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A facile approach has been developed for surface functionalization of few-layered WS_2 nanosheets with uniform gold (Au) nanoparticles (NPs) of well-defined sizes and morphologies, and their plasmonic properties were evaluated using crystal violet as a testing analyte via Raman spectroscopy. Decoration of Au NPs have been commonly performed on chemically-exfoliated WS_2 nanosheets, either via the reduction of gold (III) chloride by exposed sulfur atoms, which occur primarily at edge and defect sites,[1] or by mixing pre-formed Au NPs with suspended WS_2 nanosheets.[2] However, these techniques fall short of providing satisfactory control in the size and the shape of Au NPs, and they are yet able to produce hybrid nanocomposites with desirable plasmonic properties. Furthermore, direct functionalization of Au NPs on the WS_2 basal plane remains elusive. Homogeneous deposition of gold nanoparticles on WS_2 nanosheets was achieved by varying the ratio of hydrogen tetrachloroaurate and dopamine, in which dopamine serves as both an anchor and a reducing agent. The as-prepared nanocomposites were characterized using ultraviolet–visible spectroscopy, X-ray diffraction, and transmission electron microscopy. Moreover, the amplification of Raman signals of crystal violet was investigated at different excitation wavelengths to study the effect of the laser resonance with the absorption band of each dye and with the synergistic oscillation modes of gold nanoparticle-decorated WS_2 heterostructures. Our results demonstrate that controlled decoration of Au NPs on ultrathin transition metal chalcogenides (TMCs) is a robust strategy to develop highly-efficient and flexible substrates for surface-enhanced Raman scattering (SERS)-based sensors (as shown in Fig.1).

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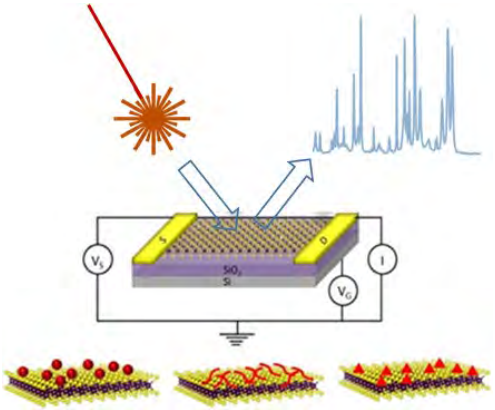

Figure 1: Gold nanoparticle-decorated two dimensional ultrathin TMCs for SERS-based chemical sensing

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Ground state of an anisotropic 2D exciton and magnetoexciton in phosphorene monolayer and bilayer

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This work investigates the anisotropic properties of the ground state of excitons in a two-dimensional (2D) atomically-thin monolayer [1], with a specific example of black phosphorus monolayer (phosphorene), as well as magnetoexcitons [2] (excitons on a bilayer in transverse magnetic field) arising due to the anisotropic effective mass in the considered material [3]. Within the variational approach, we calculate the ground-state energy and wave functions depending on the mass anisotropy parameter introduced to characterize the system, on the interlayer distance and strength of the external magnetic field (see Fig. 1), and discuss possible implications on the collective properties of excitons and magnetoexcitons in van der Waals materials.

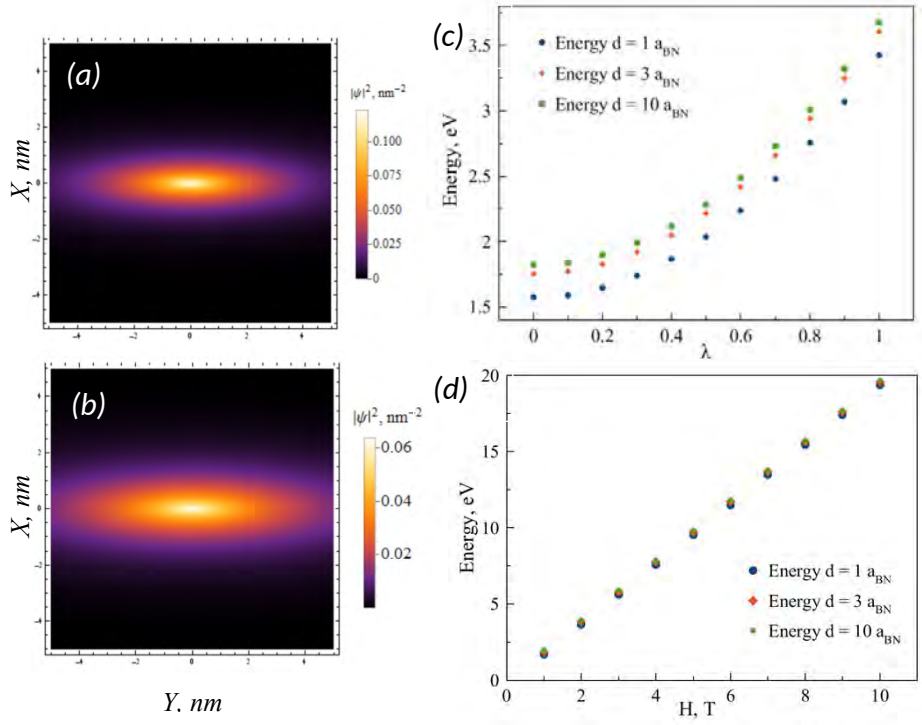

Figure 1: (a,b) Ground state wave function profile for anisotropic exciton in a monolayer of phosphorene (a) in vacuum, (b) encapsulated in hBN medium. (c,d) Ground state energy of the anisotropic magnetoexciton in an anisotropic bilayer for different interlayer distances as marked, (c) dependent on the mass anisotropy parameter $\lambda = \sqrt{\mu_x / \mu_y}$, (d) for phosphorene bilayer, dependent on the magnetic field.

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Excitonic Effects and Non-trivial Spin Polarization at Filling Factor of 3/2

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The even-denominator fractional states can be described in terms of the interaction of a pair of composite fermions with the formation of composite bosons [1]. Surprisingly, 5/2 quantum Hall state was discovered prior to 3/2 state which is more simple and stable at first glance. Recent magnetotransport experiments showed similar results in GaAs/AlGaAs heterostructures with the modified edge states [2].

We used optical methods of photoluminescence, resonance light reflection, and photo-induced light reflection as a probe. We observed non-trivial spin polarization of the ground state near the filling factor of 3/2. Furthermore, the lifetime of spin excitations reaches 10 us [3]. Spin excitations also change the luminescence spectrum drastically, possibly due to nontrivial dispersion at fractional filling factor. We also propose numerical simulation of the ground state and spin excitations at filling factor of 3/2.

V. A. K. and I. V. K. thank Basic Research program of HSE for computational facilities. V. A. K., L. V. K., and A. S. Z. thank Russian Science Foundation (project no. 18-12-00246).

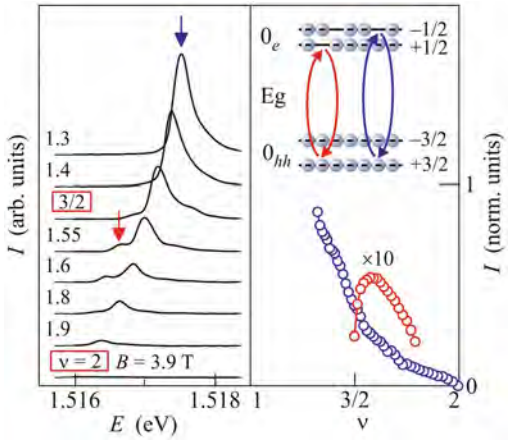

Figure 1: (Left panel) Resonance light scattering spectra including optical transitions from the lowest Landau level of the heavy hole valence band (0hh) to the lowest Landau level of the conduction band (0e) of the quantum well at different filling factors ν for the twodimensional electron system. (Right panel) Relative integral intensities of the resonant reflection lines from the states of the lowest Landau level versus the electron filling factor. The diagram shows the corresponding optical transitions.

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Anomalous Screening in Narrow-Gap Carbon Nanotubes

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The Coulomb interaction between electrons in metallic (armchair) carbon nanotubes turns out to be surprisingly strong according to first-principles simulations [1], well beyond the expectation of current theoretical models [2-3]. In this work, we develop a full theory of screening in narrow-gap carbon nanotubes by combining first-principles and model calculations. Starting from a two-band model, we make use of the supercell technique [4] to derive the RPA dielectric function for narrow-gap tubes of any size and chirality, validating it with selected first-principles studies. We find that the anomalous screening is linked to the full three-dimensional topology of the tube, which is missed by effective-mass approaches. A correct description of the screening is essential to correctly assess possible electronic instabilities of nominally metallic carbon nanotubes, such as those leading to the excitonic insulator state, proposed in the sixties and recently claimed [1] for armchair tubes.

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Efficient single-photon sources of red light based on a waveguide photonic nanoantenna with an InAs/AlGaAs quantum dot

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In the last decades, a lot of attention has been paid to development of the sources of quantum light such as single-photon emitters possessing non-classical photon statistics and sources of entangled pairs of single photons. These devices are key elements for the systems of quantum cryptography, information teleportation, and quantum computing. Semiconductor self-organized quantum dots (QDs) are promising candidates due to their ability to be integrated with electronic devices, high quantum efficiency and small emission linewidth. InAs/AlGaAs QDs attracted a considerable attention because of their possible application as single photon sources in a wide wavelength range including the spectral region of the highest sensitivity of modern silicon single-photon avalanche photodiodes (600-700 nm). In particular, Polimeni et. al. [1] found that the QDs luminescence can be tuned over the wide wavelength range from 640 to 1000 nm only by varying the growth conditions. However, to the best of our knowledge, there have been only few reports about single photon emission from the InAs/AlGaAs QDs [2, 3].

Here, we investigate the possibility of creating an efficient single-photon source for the red part of the spectrum with wavelengths shorter than 700 nm. The proposed source is based on InAs/AlGaAs QDs grown by molecular beam epitaxy on GaAs (001) substrates, using the Stranski-Krastanow growth mechanism. We investigated the statistics of correlations of photons emitted by a single photonic nanostructure in which an InAs/AlGaAs QD was placed in a columnar (nearly cylindrical) AlGaAs waveguide with a variable cross section. Such a waveguide operates essentially as a photonic nanoantenna coupling the QD emission to far optical field. By properly choosing the parameters of the waveguide (base diameter, refractive index, and height), it is possible to increase the efficiency of radiation extraction from the QDs up to 90% [4]. The use of such nanoantennas allowed us to implement a bright source of single photons with a wavelength shorter than 700 nm and average intensity exceeding 16 MHz at the temperature of 10 K. The emission properties of single quantum dots were investigated by using micro-photoluminescence setup. The μ-PL measurements revealed the low QDs density (less than 10^{10} cm^{-2}), which is perfectly suitable for the creation of single photon sources based on emission of single QDs. For the confirmation of single photon statistics, the second-order correlation function $g^{(2)}(\tau)$ was measured and analyzed.

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Magnetic phase diagram of a spin $S = 1/2$ antiferromagnetic two-leg ladder with in the presence of modulated along legs Dzyaloshinskii-Moriya interaction

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We study the ground-state magnetic phase diagram of a spin $S = 1/2$ antiferromagnetic two-leg ladder in the presence of period two lattice units modulated, Dzyaloshinskii-Moriya (DM) interaction along the legs. We consider the case of collinear DM vectors and strong rung exchange and magnetic field. In this limit we map the initial ladder model onto the effective spin $\sigma = 1/2$ XXZ chain and study the latter using the continuum-limit bosonization approach.

We identified four quantum phase transitions and corresponding critical magnetic fields, which mark transitions from the spin gapped regimes into the gapless quantum spin-liquid regimes. In the gapped phases the magnetization curve of the system shows plateaus at magnetisation $M = 0$ and to its saturation value per rung $M = M_{sat} = 1$. We have shown that the very presence of alternating DM interaction leads to opening of a gap in the excitation spectrum at magnetization $M = 0.5M_{sat}$. The width of the magnetization plateau at $M = 0.5M_{sat}$, is determined by the associated with the dynamical generation of a gap in the spectrum is calculated and is shown that its length scales as $(D_0D_1/J^2)^\alpha$ where D_0, D_1 are uniform and staggered components of the DM term, J is the intraleg exchange and $\alpha \leq 3/4$ and weakly depends on the DM couplings.

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Study of Resistive Switching Effect in Si+W+ZrO_2+HfO_2+Mo+Al Nanostructure

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Nowadays, one of the most important issues in micro and nanoelectronics is the development of the new type of non-volatile memory as floating-gate MOSFET flash memories are not capable of providing the higher storage capacities. This problem has caused the necessity to develop the device of new type with suitable physical properties to replace the floating-gate based flash memory. The latest research in micro and nanoelectronics has revealed the opportunity for the new type of non-volatile memory element production on the basis of transition metal oxides and dioxides, named the memristor. A typical memristor is built on the nanosize (<70nm) transition metal oxide and dioxide films (TiO_x, TiO_2, HfO_x, HfO_2, ZrOx, ZrO_2) sandwiched between two metallic electrodes [1]. Materials of this class are interesting because their *d* orbitals are not occupied by electrons. The uniqueness of the memristor is based on the motion of ions under the influence of an electric field. The voltage applied causes the change in the device resistance. After terminating the power supply, the memristor remembers the amount of charge that has previously flowed through it. This means that it can retain memory without power.

Traditional technological processes of the fabrication of oxide layers are carried out at high (1300K) temperatures. High-temperature processing results in the increased surface roughness, spread of diffusion regions, worsened adhesion, also hindering the controlled growth of the oxide layers. Because of many negative effects caused by the high-temperature technology it is highly desirable to decrease the process implementation temperature.

In our work, the low-temperature technology is considered for the metal-oxide-semiconductor (MOS) structure fabrication. We study the influence of the pulse photon treatment (PPT) and annealing in the N_2 ambient on the physical characteristics of dioxide layers, followed by the fabrication of the memristor with improved physical properties on the basis of the transition metal dioxides, followed by the analysis of the electro-physical and structural characteristics of the device fabricated. Our low-temperature technology is the reactive magnetron sputtering, which allows us to decrease the proccesing temperature down to the range of 473-750 K [2].

It has been shown that the PPT and annealing in the N_2 ambient significantly improve the electro-physical characteristics of the dioxide layers. As a result of additional treatments, transition metal dioxides with improved physical properties were obtained and used to improve the electro-physical characteristics of the memristor. Nanostructures of Al+Si+ZrO2+HfO2+Al were fabricated on p-type silicon wafer substrates using low-temperature reactive magnetron sputtering [3]. Various measurements are conducted to study their electro-physical and structural characteristics. Dioxide layers with improved properties were then used in the Si+W+ZrO2+HfO2+Mo+Al metal-insulator-metal structure to study the resistive switching effect.

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Trions and Biexcitons in core/shell nanowires

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A study of the trion and biexciton in a nanowire (NW) in the framework of the effective-mass model is presented. We consider the formation of trions and biexcitons under the action of both the lateral confinement and the localization potential. The analytical expressions for the binding energy and eigenfunctions of the trion and biexciton are obtained and expressed by means of matrix elements of the effective one-dimensional cusp-type Coulomb potentials whose parameters are determined self-consistently by employing eigenfunctions of the confined electron and hole states. Our calculations for the ZnO/ZnMgO, CdSe/ZnS and CdSe/CdS core/shell cylindrical shaped NWs show that the trion and biexciton binding energy in NWs are size-dependent and for the same input parameters the biexciton binding energy in NWs is always larger than the binding energy of the trion. The trion and biexciton remain stable in CdSe/ZnS NW with the increase of the dielectric shell, while in ZnO/ZnMgO NW they become unstable when the surrounding dielectric shell exceeds 2.5 nm and 2 nm for each, respectively. The associative ionization of biexciton antibonding states into trion bonding states that leads to the formation of trions is studied. Based on the results for size dependence of biexciton binding energy and probability associative ionization an optimal radius for optoelectronic application NW is suggested [1].

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