



Tnano20: International Workshop on Nanotechnology

*Initially planned to take place in
Tbilisi, Republic of Georgia*

Now purely virtual via Zoom

October 5-8, 2020

Home Page: <https://nanoten.com/conf-org/Tnano20/>

Book of Abstracts





Program

Social Program



Virtual Cheers! (bring your drink to the Zoom camera)



Virtual banquet (eat at home)



Virtual excursion (online photo/video show)

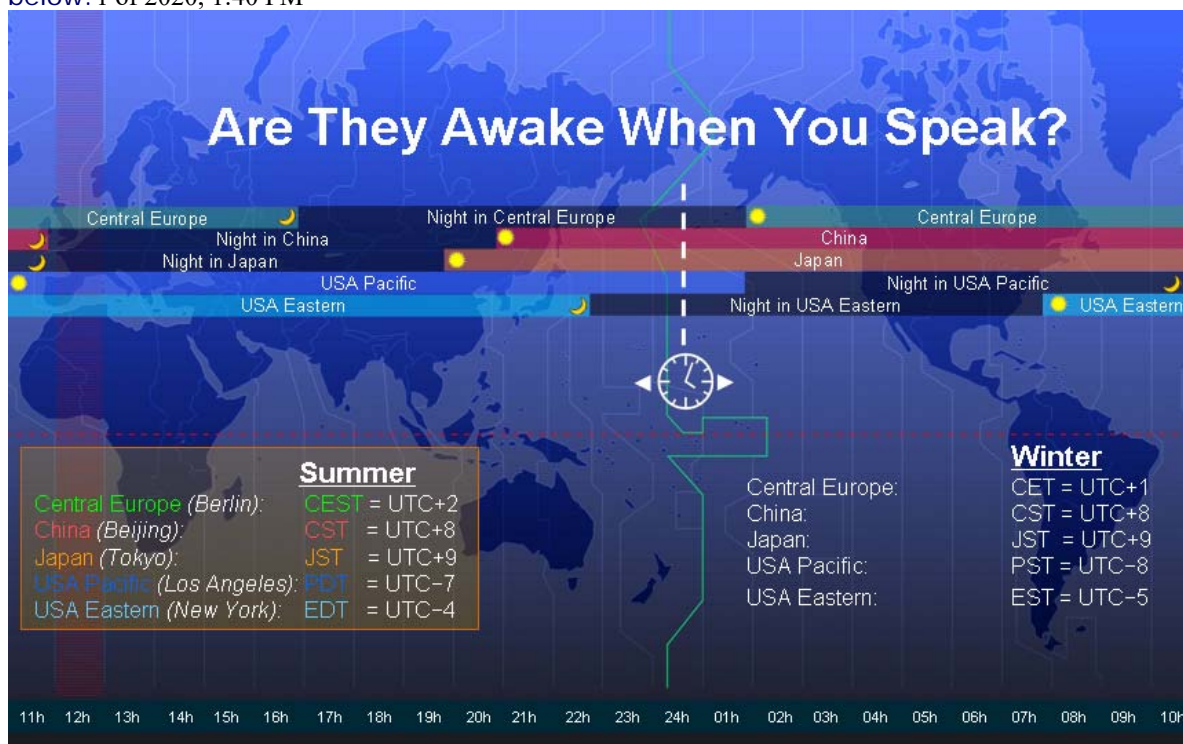
Technical Program

- The key purpose of a **workshop** is to share and **discuss** information. Therefore, discussion periods are generously long. Speakers are requested to adhere to the presentation duration specified below.
- The **Book of Abstracts** can be downloaded [HERE](#).
- An **Alphabetic List of Presenters, Affiliations and Abstracts** is posted [HERE](#).
- Time slots for presentations in the following program are identified by a letter (K, I, C, M) followed by a number. Most slots have a speaker, some do not. These slots can be used for focussed discussions or "breakout" sessions in "personal rooms".

Presentation duration


Presentation Type	Presentation Length	Question Period
Keynote (K)	45 minutes	15 minutes
Invited (I)	35 minutes	10 minutes
Contributed (C)	20 minutes	10 minutes
Mini-Talks (M)	10 minutes	5 minutes

The Tnano20 official date and time, used in the program below, are the **Universal Time (UTC)**. UTC stands for *Coordinated Universal Time*, formerly known as *Greenwich Mean Time (GMT)*. Locate **YOUR TIME ZONE**, its **CODE**, and its relation to UTC in the map below: 1 of 2020, 1:40 PM



October 5, 2020


Chairs: David Tománek, Igor Bondarev

Central Europe	CEST	13:45-14:00	14:00-15:00	15:00-15:45	15:45-16:00	16:00-16:45	16:45-17:30
China	CST	19:45-20:00	20:00-21:00	21:00-21:45	21:45-22:00	22:00-22:45	22:45-23:30
Japan	JST	20:45-21:00	21:00-22:00	22:00-22:45	22:45-23:00	23:00-23:45	23:45-00:30*
USA-West	PDT	04:45-05:00	05:00-06:00	06:00-06:45	06:45-07:00	07:00-07:45	07:45-08:30
USA-East	EDT	07:45-08:00	08:00-09:00	09:00-09:45	09:45-10:00	10:00-10:45	10:45-11:30
Universal Time	UTC	11:45-12:00	12:00-13:00	13:00-13:45	13:45-14:00	14:00-14:45	14:45-15:30
		Opening Ceremony	K01: Pablo Jarillo-Herrero	I01: David Tománek		I02: Frank Koppens	I03: Katsumi Kaneko


* stands for "date change" or "next day"

Central Europe	CEST	17:30-18:15	18:15-19:00	19:00-19:45	19:45-20:30	20:30-21:15	21:15-21:30
China	CST	23:30-00:15*	00:15-01:00*	01:00-01:45*	01:45-02:30*	02:30-03:15*	03:15-03:30*
Japan	JST	00:30-01:15*	01:15-02:00*	02:00-02:45*	02:45-03:30*	03:30-04:15*	04:15-04:30*
USA-West	PDT	08:30-09:15	09:15-10:00	10:00-10:45	10:45-11:30	11:30-12:15	12:15-12:30
USA-East	EDT	11:30-12:15	12:15-13:00	13:00-13:45	13:45-14:30	14:30-15:15	15:15-15:30
Universal Time	UTC	15:30-16:15	16:15-17:00	17:00-17:45	17:45-18:30	18:30-19:15	19:15-19:30
		I04: Fengnian Xia		I05: Qiaoxia Xing	I06: Hui Deng	I07: Chern Chuang	

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Central Europe	CEST	21:30-22:15	22:15-23:00	23:00-23:45	23:45-00:00	00:00-00:45*	00:45-01:30*
China	CST	03:30-04:15*	04:15-05:00*	05:00-05:45*	05:45-06:00*	06:00-06:45*	06:45-07:30*
Japan	JST	04:30-05:15*	05:15-06:00*	06:00-06:45*	06:45-07:00*	07:00-07:45*	07:45-08:30*
USA-West	PDT	12:30-13:15	13:15-14:00	14:00-14:45	14:45-15:00	15:00-15:45	15:45-16:30
USA-East	EDT	15:30-16:15	16:15-17:00	17:00-17:45	17:45-18:00	18:00-18:45	18:45-19:30
Universal Time	UTC	19:30-20:15	20:15-21:00	21:00-21:45	21:45-22:00	22:00-22:45	22:45-23:30
		I08: Vasili Perebeinos	I09: Igor Bondarev	I10: Sergei Tretiak		I11: Igor Popov	I12: Vinod Menon

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Central Europe	CEST	01:30-02:15*	02:15-02:30*	02:30-03:15*	03:15-04:00*	04:00-04:45*
China	CST	07:30-08:15*	08:15-08:30*	08:30-09:15*	09:15-10:00*	10:00-10:45*
Japan	JST	08:30-09:15*	09:15-09:30*	09:30-10:15*	10:15-11:00*	11:00-11:45*
USA-West	PDT	16:30-17:15	17:15-17:30	17:30-18:15	18:15-19:00	19:00-19:45
USA-East	EDT	19:30-20:15	20:15-20:30	20:30-21:15	21:15-22:00	22:00-22:45
Universal Time	UTC	23:30-00:15*	00:15-00:30*	00:30-01:15*	01:15-02:00*	02:00-02:45*
		I 13: Oleg L. Berman		I 14: Wang Yao	I 15: Kin Fai Mak	I 16: Junhao Lin

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Opening Ceremony

11:45-12:00
UTC

OPENING CEREMONY AND
GENERAL INFORMATION

Magic Carbon

12:00-13:00 K01: **Pablo JARILLO-
HERRERO**
UTC

MAGIC-ANGLE GRAPHENE: CORRELATIONS,
SUPERCONDUCTIVITY, AND BEYOND

13:00-13:45 I01: **David TOMÁNEK**
UTC

MAGIC OF CARBON ON THE NANOSCALE

13:45-14:00
UTC



COFFEE BREAK

14:00-14:45 I02: **Frank KOPPENS**
UTC

STACKING AND TWISTING GRAPHENE AND
OTHER 2D MATERIALS FOR QUANTUM NANO-
OPTOELECTRONICS

14:45-15:30 I03: **Katsumi KANEKO**
UTC

MORPHOLOGICALLY DESIGNED NOVEL
NANOCARBON MATERIALS DERIVED FROM
HIGHLY STABLE SWCNT INKS

Applications of Graphene

15:30-16:15 I04: **Fengnian XIA**
UTC

STRONG MID-INFRARED PHOTO RESPONSE IN
TWISTED BILAYER GRAPHENE

16:15-17:00
UTC



LUNCH BREAK

17:00-17:45 I05: **Qiaoxia XING**
UTC

TUNABLE GRAPHENE SPLIT-RING RESONATORS

Light-Matter Interaction


17:45-18:30 UTC	I06: Hui DENG	COHERENT LIGHT-MATTER INTERACTIONS IN 2D SEMICONDUCTORS
18:30-19:15 UTC	I07: Chern CHUANG	UNIVERSAL SCALING OF THE ANISOTROPIC DISPERSION IN 2D EXCITONIC SYSTEMS AND ITS SPECTROSCOPIC SIGNATURES
19:15-19:30 UTC		COFFEE BREAK
19:30-20:15 UTC	I08: Vasili PEREBEINOS	DOPING DEPENDENCE OF TRIONS AND OPTICAL SPECTRA IN MoS ₂
20:15-21:00 UTC	I09: Igor BONDAREV	CRYSTAL PHASES OF CHARGED INTERLAYER EXCITONS IN VAN DER WAALS HETEROSTRUCTURES
21:00-21:45 UTC	I10: Sergei TRETIAK	HYBRID 2D AND 3D NANOSTRUCTURED PEROVSKITES: FROM UNDERSTANDING FUNDAMENTAL PHYSICS TO OPTOELECTRONIC APPLICATIONS
21:45-22:00 UTC		DINNER BREAK
22:00-22:45 UTC	I11: Igor POPOV	TWO FACES OF A DOUBLE WELL: MULTIFUNCTIONAL DEVICE BASED ON A TI ₂ O MONOLAYER AND MAGNETO-MECHANICAL SWITCH BASED ON A MXENE NANOTUBE
22:45-23:30 UTC	I12: Vinod M. MENON	STRONG LIGHT-MATTER COUPLING IN 2D ATOMIC CRYSTALS
23:30-00:15* UTC	I13: Oleg L. BERMAN	PHASE TRANSITIONS AND EXCITON SUPERFLUIDITY IN DOUBLE LAYERS OF NOVEL TWO-DIMENSIONAL NANOMATERIALS
00:15-00:30* UTC		COFFEE BREAK

Moiré Magic



00:30-01:15* UTC	I14: Wang YAO	BERRY PHASES IN THE MOIRÉ PATTERNS OF TWISTED TMD BILAYERS WITH UNIFORM AND NON-UNIFORM STRAINS
01:15-02:00* UTC	I15: Kin Fai MAK	STRONGLY CORRELATED PHASES OF MATTER IN SEMICONDUCTOR MOIRÉ SUPERLATTICES
02:00-02:45* UTC	I16: Junhao LIN	DEFECTS AND DEFECT DYNAMICS IN NOVEL 2D MATERIALS

October 6, 2020


Chairs: Roland Kawakami, Frank Koppens, Vasili Perebeinos, David Tománek

Central Europe	CEST	13:45-14:00	14:00-15:00	15:00-15:45	15:45-16:00	16:00-16:45	16:45-17:30
China	CST	19:45-20:00	20:00-21:00	21:00-21:45	21:45-22:00	22:00-22:45	22:45-23:30
Japan	JST	20:45-21:00	21:00-22:00	22:00-22:45	22:45-23:00	23:00-23:45	23:45-00:30*
USA-West	PDT	04:45-05:00	05:00-06:00	06:00-06:45	06:45-07:00	07:00-07:45	07:45-08:30
USA-East	EDT	07:45-08:00	08:00-09:00	09:00-09:45	09:45-10:00	10:00-10:45	10:45-11:30
Universal Time	UTC	11:45-12:00	12:00-13:00	13:00-13:45	13:45-14:00	14:00-14:45	14:45-15:30
		Opening Remarks	K02: Philip Kim	I17: Roland Kawakami		I18: Yoshihiro Iwasa	I19: Klaus Ziegler

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China	CST	23:30-00:15*	00:15-01:00*	01:00-01:45*	01:45-02:30*	02:30-03:15*	03:15-03:30*
Japan	JST	00:30-01:15*	01:15-02:00*	02:00-02:45*	02:45-03:30*	03:30-04:15*	04:15-04:30*
USA-West	PDT	08:30-09:15	09:15-10:00	10:00-10:45	10:45-11:30	11:30-12:15	12:15-12:30
USA-East	EDT	11:30-12:15	12:15-13:00	13:00-13:45	13:45-14:30	14:30-15:15	15:15-15:30
Universal Time	UTC	15:30-16:15	16:15-17:00	17:00-17:45	17:45-18:30	18:30-19:15	19:15-19:30
		I20: Maarten Biesheuvel		I21: Athanasios Chantis	Meet  Physical Review Editors		

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Central Europe	CEST	21:30-22:15	22:15-23:00	23:00-23:45	23:45-00:00	00:00-00:45*	00:45-01:30*
China	CST	03:30-04:15*	04:15-05:00*	05:00-05:45*	05:45-06:00*	06:00-06:45*	06:45-07:30*
Japan	JST	04:30-05:15*	05:15-06:00*	06:00-06:45*	06:45-07:00*	07:00-07:45*	07:45-08:30*
USA-West	PDT	12:30-13:15	13:15-14:00	14:00-14:45	14:45-15:00	15:00-15:45	15:45-16:30
USA-East	EDT	15:30-16:15	16:15-17:00	17:00-17:45	17:45-18:00	18:00-18:45	18:45-19:30
Universal Time	UTC	19:30-20:15	20:15-21:00	21:00-21:45	21:45-22:00	22:00-22:45	22:45-23:30
		I24	I25	I26: Philippe Jund		M27: Vyacheslav Semenenko	I28: Kwanpyo Kim

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Central Europe	CEST	01:30-02:15*	02:15-02:30*	02:30-03:15*	03:15-04:00*	04:00-04:45*
China	CST	07:30-08:15*	08:15-08:30*	08:30-09:15*	09:15-10:00*	10:00-10:45*
Japan	JST	08:30-09:15*	09:15-09:30*	09:30-10:15*	10:15-11:00*	11:00-11:45*
USA-West	PDT	16:30-17:15	17:15-17:30	17:30-18:15	18:15-19:00	19:00-19:45
USA-East	EDT	19:30-20:15	20:15-20:30	20:30-21:15	21:15-22:00	22:00-22:45
Universal Time	UTC	23:30-00:15*	00:15-00:30*	00:30-01:15*	01:15-02:00*	02:00-02:45*
		I 29: Jinying Zhang		I 30: Huaihong Guo	I 31: Jie Guan	I 32: Hugh Churchill

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Superconductivity, Magnetism, and Charge Interaction in 2D

11:45-12:00 UTC			OPENING REMARKS
12:00-13:00 UTC	K02:	Philip KIM	INDUCED SUPERCONDUCTIVITY IN THE FRACTIONAL QUANTUM HALL EDGE IN GRAPHENE HETEROSTRUCTURES
13:00-13:45 UTC	I17:	Roland KAWAKAMI	2D AND TOPOLOGICAL MAGNETIC MATERIALS
13:45-14:00 UTC			COFFEE BREAK
14:00-14:45 UTC	I18:	Yoshihiro IWASA	BCS-BEC CROSSOVER IN A 2D SUPERCONDUCTOR
14:45-15:30 UTC	I19:	Klaus ZIEGLER	PAIRING TRANSITION IN INTERACTING ELECTRONIC DOUBLE LAYERS
15:30-16:15 UTC	I20:	Maarten BIESHEUVEL	ELECTROSTATIC COOLING AT ELECTROLYTE-ELECTROLYTE JUNCTIONS
16:15-17:00 UTC			LUNCH BREAK

Physical Review Session

17:00-17:45 UTC	I21:	Athanasios CHANTIS	ALL YOU WANTED TO KNOW ABOUT PUBLISHING IN PHYSICAL REVIEW JOURNALS
17:45-19:15 UTC			MEET PHYSICAL REVIEW EDITORS

Defects

21:00-21:45 UTC I26: **Philippe JUND**

DEFECTS AND THEIR INFLUENCE ON THE THERMOELECTRIC PROPERTIES OF MATERIALS: AN *AB INITIO* STUDY

21:45-22:30 UTC



DINNER BREAK

Mini-Presentations

22:30-22:45 UTC M27: **Vyacheslav SEMENENKO** SCATTERING OF PLASMONS IN CLOSELY PACKED 1D GRAPHENE STRUCTURES

Non-Carbon 2D and 1D Structures

22:45-23:30 UTC I28: **Kwanpyo KIM**

NEW PHOSPHORUS STRUCTURES: FROM TYPE-II RED PHOSPHORUS TO PHOSPHORENE EDGES

23:30-00:15* UTC I29: **Jinying ZHANG**

VIOLET PHOSPHORUS AND PHOSPHORENE

00:15-00:30* UTC



COFFEE BREAK

00:30-01:15* UTC I30: **Huaihong GUO**

DOUBLE RESONANT RAMAN SCATTERING IN TMDCS

01:15-02:00* UTC I31: **Jie GUAN**


LOW-SYMMETRY TWO-DIMENSIONAL STRUCTURES WITH ANISOTROPIC HIGH CARRIER MOBILITY

02:00-02:45* UTC I32: **Hugh CHURCHILL**



QUANTUM DEVICES WITH 2D SEMICONDUCTORS AND INSULATORS

October 7, 2020

Chairs: Jeanie Lau, Frank Koppens, Eunja Kim, Young-Kyun Kwon

Central Europe	CEST	13:45-14:00	14:00-15:00	15:00-15:45	15:45-16:00	16:00-16:45	16:45-17:30
China	CST	19:45-20:00	20:00-21:00	21:00-21:45	21:45-22:00	22:00-22:45	22:45-23:30
Japan	JST	20:45-21:00	21:00-22:00	22:00-22:45	22:45-23:00	23:00-23:45	23:45-00:30*
USA-West	PDT	04:45-05:00	05:00-06:00	06:00-06:45	06:45-07:00	07:00-07:45	07:45-08:30
USA-East	EDT	07:45-08:00	08:00-09:00	09:00-09:45	09:45-10:00	10:00-10:45	10:45-11:30
Universal Time	UTC	11:45-12:00	12:00-13:00	13:00-13:45	13:45-14:00	14:00-14:45	14:45-15:30
				I33: Feng Miao		I34: Teng Yang	I35: Savas Berber


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Central Europe	CEST	17:30-18:15	18:15-19:00	19:00-19:45	19:45-20:30	20:30-21:15	21:15-21:30
China	CST	23:30-00:15*	00:15-01:00*	01:00-01:45*	01:45-02:30*	02:30-03:15*	03:15-03:30*
Japan	JST	00:30-01:15*	01:15-02:00*	02:00-02:45*	02:45-03:30*	03:30-04:15*	04:15-04:30*
USA-West	PDT	08:30-09:15	09:15-10:00	10:00-10:45	10:45-11:30	11:30-12:15	12:15-12:30
USA-East	EDT	11:30-12:15	12:15-13:00	13:00-13:45	13:45-14:30	14:30-15:15	15:15-15:30
Universal Time	UTC	15:30-16:15	16:15-17:00	17:00-17:45	17:45-18:30	18:30-19:15	19:15-19:30
		I36: Jeanie (ChunNing) Lau		I37	I38	I39	

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Central Europe	CEST	21:30-22:15	22:15-23:00	23:00-23:45	23:45-00:00	00:00-00:45*	00:45-01:30*
China	CST	03:30-04:15*	04:15-05:00*	05:00-05:45*	05:45-06:00*	06:00-06:45*	06:45-07:30*
Japan	JST	04:30-05:15*	05:15-06:00*	06:00-06:45*	06:45-07:00*	07:00-07:45*	07:45-08:30*
USA-West	PDT	12:30-13:15	13:15-14:00	14:00-14:45	14:45-15:00	15:00-15:45	15:45-16:30
USA-East	EDT	15:30-16:15	16:15-17:00	17:00-17:45	17:45-18:00	18:00-18:45	18:45-19:30
Universal Time	UTC	19:30-20:15	20:15-21:00	21:00-21:45	21:45-22:00	22:00-22:45	22:45-23:30
		I40	I41	I42		I43	I44

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Central Europe	CEST	01:30-02:15*	02:15-02:30*	02:30-03:15*	03:15-04:00*	04:00-04:45*
China	CST	07:30-08:15*	08:15-08:30*	08:30-09:15*	09:15-10:00*	10:00-10:45*
Japan	JST	08:30-09:15*	09:15-09:30*	09:30-10:15*	10:15-11:00*	11:00-11:45*
USA-West	PDT	16:30-17:15	17:15-17:30	17:30-18:15	18:15-19:00	19:00-19:45
USA-East	EDT	19:30-20:15	20:15-20:30	20:30-21:15	21:15-22:00	22:00-22:45
Universal Time	UTC	23:30-00:15*	00:15-00:30*	00:30-01:15*	01:15-02:00*	02:00-02:45*
		I45		I46: Young-Kyun Kwon	I47: Bo Song	I48: Eunja Kim

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Non-Carbon 2D Devices

13:00-13:45 UTC	I33: Feng MIAO	2D VAN DER WAALS HETEROSTRUCTURES FOR EMERGING DEVICE APPLICATIONS
13:45-14:00 UTC		COFFEE BREAK
14:00-14:45 UTC	I34: Teng YANG	GATE TUNABLE ANISOTROPY IN 2D GATE
14:45-15:30 UTC	I35: Savaş BERBER	DEVICE APPLICATIONS OF MXENES
15:30-16:15 UTC	I36: Chun Ning (Jeanie) LAU	TUNABLE SPIN-ORBIT COUPLING IN A HIGH MOBILITY FEW-LAYER SEMICONDUCTOR
16:15-17:00 UTC		LUNCH BREAK

Other Nanostructures

00:30-01:15* UTC	I46: Young-Kyun KWON	UNUSUALLY STRONG "HIDDEN" RASHBA EFFECTS IN Si_2Bi_2
01:15-02:00* UTC	I47: Bo SONG	CELL POLARITON: A QUANTUM STATE IN THE MYELIN SHEATH OF A NERVE
02:00-02:45* UTC	I48: Eunja KIM	SEMICONDUCTING LAYERED TRANSITION-METAL DICHALCOGENIDES: INSIGHTS FROM FIRST-PRINCIPLES

October 8, 2020

Central Europe	CEST	15:00-16:30	16:30-17:00
China	CST	21:00-22:30	22:30-23:00
Japan	JST	22:00-23:30	23:30-00:00
USA-West	PDT	06:00-07:30	07:30-08:00
USA-East	EDT	09:00-10:30	10:30-11:00
Universal Time	UTC	13:00-14:30	14:30-15:00
		David Tománek and Colleagues	Closing Ceremony

Closing Session

13:00-14:30
UTC **David TOMÁNEK and Colleagues**

FROM GRADUATION TO RETIREMENT:
DAVID TOMÁNEK – A HUMAN AND A SCIENTIST

14:30-15:00
UTC

CLOSING CEREMONY

MAGIC-ANGLE GRAPHENE: CORRELATIONS, SUPERCONDUCTIVITY, AND BEYOND

Pablo JARILLO-HERRERO

Department of Physics, M.I.T., Cambridge, MA 02138, USA
pjarillo@mit.edu

The understanding of strongly-correlated quantum matter has challenged physicists for decades. Such difficulties have stimulated new research paradigms, such as ultra-cold atom lattices for simulating quantum materials. In this talk I will present a new platform to investigate strongly correlated physics, based on graphene moiré superlattices. In particular, I will show that when two graphene sheets are twisted by an angle close to the theoretically predicted ‘magic angle’, the resulting flat band structure near the Dirac point gives rise to a strongly-correlated electronic system. These flat bands exhibit half-filling insulating phases at zero magnetic field, which we show to be a correlated insulator arising from electrons localized in the moiré superlattice. Moreover, upon doping, we find electrically tunable superconductivity in this system, with many characteristics similar to high-temperature cuprate superconductivity. These unique properties of magic-angle twisted bilayer graphene open up a new playground for exotic many-body quantum phases in a 2D platform made of pure carbon and without magnetic field. The easy accessibility of the flat bands, the electrical tunability, and the bandwidth tunability through twist angle may pave the way towards more exotic correlated systems, such as quantum spin liquids or correlated topological insulators.

MAGIC OF CARBON ON THE NANOSCALE

David TOMÁNEK

Physics and Astronomy Department, Michigan State University, East Lansing, Michigan, USA
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With its complex behavior, which is becoming unveiled by *ab initio* DFT calculations, carbon fills a unique place in the periodic table. Both graphene and related nanometer-wide carbon nanotubes (CNTs) are unusually stable both mechanically and thermally. A structure consisting of graphite oxide, a fleece of CNTs, and strong carbon fabric layers may become the long-sought magic membrane capable of filtering and desalinating water [1] without the shortcoming of commercial reverse osmosis membranes. CNTs may also be used as magic autoclaves and nanoreactors capable of transforming enclosed NbCl_3 molecules Nb metal [2]. The concerted transformation process is accelerated by the catalytic activity of the CNT that lowers activation barriers and the conversion temperature to below the high melting temperature $T_M=2,750$ K of Nb. A third example of apparent magic involves the twist degree of freedom in layered 2D structures, which changes the Moiré pattern shown in Fig. 1. Recent evidence suggests that the twisted bilayer graphene (TBLG) develops a flat band near the magic twist angle value $\theta_m \approx 1.08^\circ$, which is separated by gaps from conduction and valence states. This behavior can not be studied by standard band structure theory methods, but parameterized models allow quantitative description of electronic structure changes [3] including their dependence on shear [3].

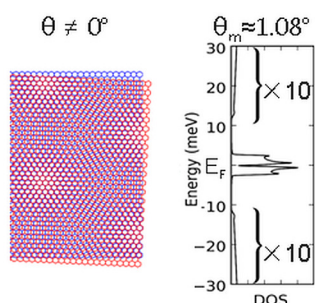


Figure 1. Unusual changes in the electronic structure of twisted bilayer graphene near the magic twist angle $\theta_m \approx 1.08^\circ$.

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STACKING AND TWISTING GRAPHENE AND OTHER 2D MATERIALS
FOR QUANTUM NANO-OPTOELECTRONICS

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Two-dimensional (2D) materials offer extraordinary potential for control of light and light-matter interactions at the atomic scale. In this talk, we will show a new toolbox to exploit the collective motion of light and charges as a probe for topological, hyperbolic and quantum phenomena.

We twist or nanostructure heterostructures of 2D materials that carry optical excitations such as excitons, plasmons or hyperbolic phonon polaritons. Nanoscale optical techniques such as near-field optical microscopy reveal with nanometer spatial resolution unique observations of topological domain wall boundaries, hyperbolic phononic cavities [1], and interband collective modes in charge neutral twisted-bilayer graphene near the magic angle [2]. The freedom to engineer these so-called optical and electronic quantum metamaterials [3] is expected to expose a myriad of unexpected phenomena.

Intriguingly, we define nanoscale phonon polaritonic cavities, where the resonances are not associated to the eigenmodes of the cavity. Rather, they are multi-modal excitations whose reflection is greatly enhanced due to the interference of constituent modes. We will also show a new type of graphene-based magnetic-resonance that we use to realize single, nanometric-scale cavities of ultra-confined acoustic graphene plasmons [4]. We reach record-breaking mode volume confinement factors of $\approx 5 \cdot 10^{-10}$. This AGP cavity acts as a Mid-infrared nanoantenna, which is efficiently excited from the far-field, and electrically tunable over an ultra-broadband spectrum. Finally, we present near-unity light absorption in a monolayer WS₂ van der Waals heterostructure cavity [5].

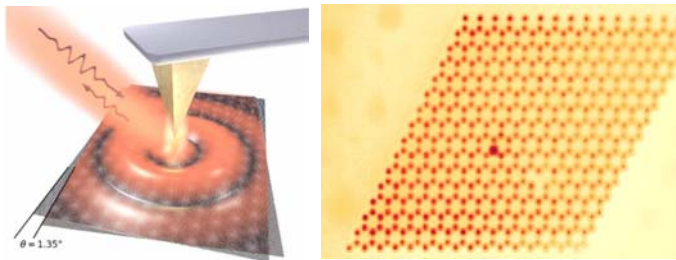


Figure 1. Collective excitations in twisted bilayer graphene. (Left) Illustration of the scattering-type scanning near-field microscopy. (Right) Image of the near-field amplitude obtained by scanning the AFM tip and recording the photodetector signal.

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MORPHOLOGICALLY DESIGNED NOVEL NANOCARBON MATERIALS DERIVED FROM
HIGHLY STABLE SWCNT INKS

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Nanoporous carbon consists of nanoscale disordered graphene units and also has a relatively high electrical conductivity. When ions are confined in the extremely narrow carbon nanopores, they induce image charges on defective carbon walls, thus reducing the ion-ion Coulomb repulsion [1]. This effect provides new insight into high-performance supercapacitors [2].

There is need for an efficient dispersant that would separate bundled SWCNTs. We have developed a Zn-Al sol-gel dispersant [3] as an alternative to widely used surfactants. The Zn-Al dispersant can be more easily removed from SWCNTs than surfactants. Then, we can uniformly deposit SWCNTs on PET [4] and flexible glass [5], resulting in a highly conductive film with transparency in the near UV region in the range of 80–90% that is temperature independent up to ≈ 600 K. The thermal stability of the SWCNT film on flexible glass exceeds that of ITO [5]. Our approach provides also SWCNT inks capable of forming free-standing SWCNT films, which give an excellent support for Pt nanoparticles used in fuel cells and SWCNT nets [6].

The Zn-Al dispersant enables to prepare stress sensors based on creased SWCNTs encapsulated in polydimethylsiloxane (PDMS) with non-fluorinated water-repellant coating. The compact design and superior water resistance of the sensor, along with its appealing linear response and large stretchability, demonstrates the scalability of such sensors applications [7]. These sensors may be combined with flexible electrodes operating in aqueous environment.

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STRONG MID-INFRARED PHOTORESPONSE IN TWISTED BILAYER GRAPHENE

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Twisted bilayer graphene has recently been extensively investigated due to its unusual physical properties. In this talk, we will discuss its infrared optical properties and its potential in mid-infrared light detection. We first show that the folding of the Brillouin zone leads to enhanced density of states and strong mid-infrared light absorption, which are tunable by the twist angle. Furthermore, we reveal the significance of the formation of superlattice bandgap. Strong mid-infrared photoresponse is observed when the Fermi-level is within the superlattice bandgap. On the contrary, when the superlattice bandgap is vanished, the photoresponse is minimized. Our demonstration provides an alternative pathway towards the realization of high performance mid-infrared photodetectors.

TUNABLE GRAPHENE SPLIT-RING RESONATORS

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A split-ring resonator is a prototype of a meta-atom in metamaterials. Although noble metal-based split ring resonators have been extensively studied, to date, there is no experimental demonstration of split-ring resonators made from graphene, an emerging intriguing plasmonic material. Here, we experimentally demonstrate graphene split-ring resonators with deep subwavelength (about one hundredth of the excitation wavelength) magnetic dipole response in the terahertz regime. Meanwhile, the quadrupole and electric dipole are observed, depending on the incident light polarization. All modes can be tuned via chemical doping or stacking multiple graphene layers. The strong interaction with surface polar phonons of the SiO₂ substrate also significantly modifies the response. Finite-element frequency-domain simulations nicely reproduce experimental results. Our study moves one stride forward toward the multifunctional graphene metamaterials, beyond simple graphene ribbon or disk arrays with electrical dipole resonances only.

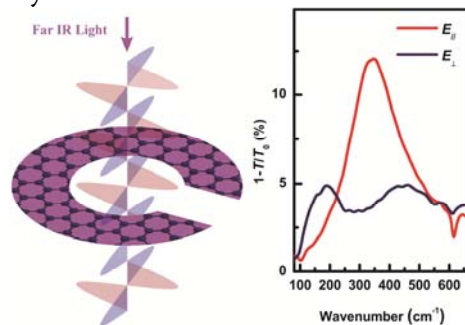


Figure 1. Split ring resonator with normal incident polarized far-infrared radiation (left), typical extinction spectra of an SRR array on Si substrate (right).

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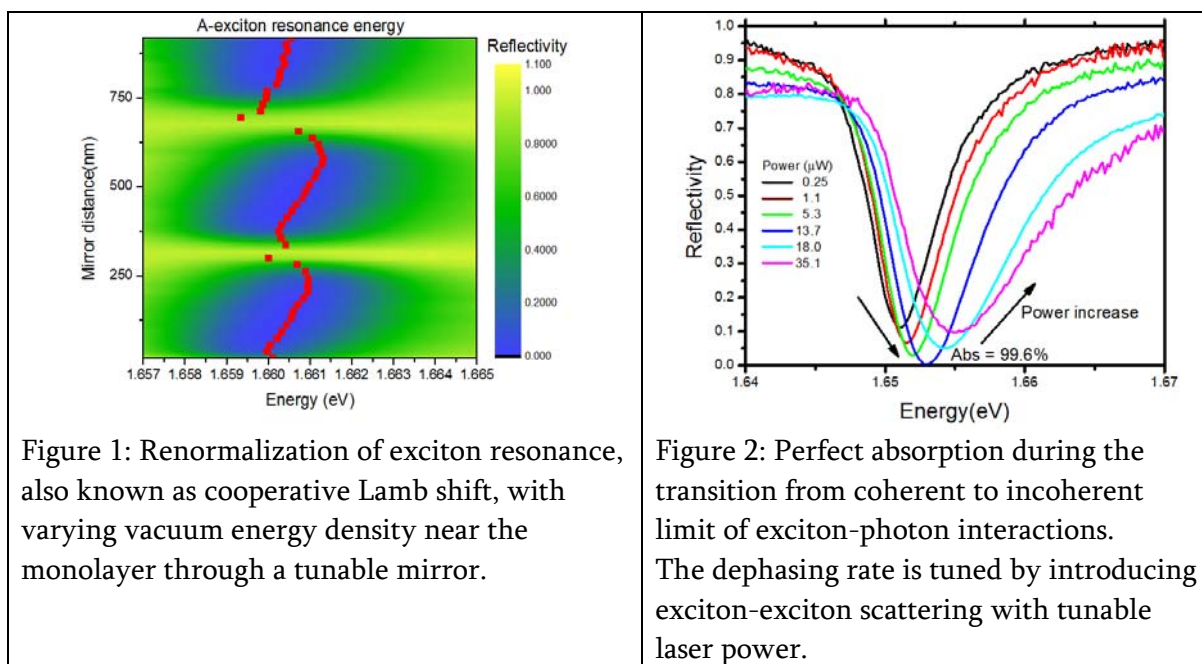
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COHERENT LIGHT-MATTER INTERACTIONS IN 2D SEMICONDUCTORS

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Van der Waals semiconductors feature excitons with exceptionally strong exciton-photon interactions. We discuss here the possibility to tune between incoherent and coherent regimes of exciton-photon interaction in monolayer transitional metal dichalcogenides (TMDs) using a simple mirror. Coherent interaction between excitons and free-space light field can be established, without a cavity, allowing direct observation of cooperative Lamb shift of the excitons [1] (Fig. 1), diminishing absorption in coherent limit, and perfect absorption under a robust critical coupling condition [2] (Fig. 2). These results suggest new possibilities in sensing and precision measurements.



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UNIVERSAL SCALING OF THE ANISOTROPIC DISPERSION IN 2D EXCITONIC SYSTEMS
AND ITS SPECTROSCOPIC SIGNATURES

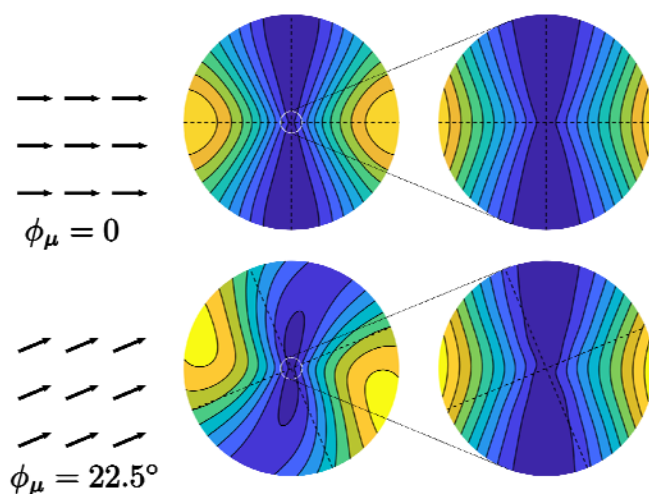
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We derive closed-form expressions for the dispersions in two-dimensional dipolar systems in the small k regime, applicable to a large class of excitonic systems such as molecular aggregates and crystals. For in-plane dipoles, the long-range dipolar contribution leads to a linearly scaling excitonic band along the direction of the dipole near the bright state, while the perpendicular direction is dispersionless up to linear order. We show that such an anisotropic dispersion relation leads to a specific scaling of the system density of states when the bright state is at the bottom of the band. Due to the insensitivity of the long-range coupling to the detailed packing conditions and molecular conformations, these universal scalings allow us to predict numerous spectroscopic signatures in the optical regime. These include absorption linewidths dependent on disorder and temperature, in addition to peak splittings in (transient) absorption spectra. The theoretical predictions of these observables are in quantitative agreement with numerical simulations of molecular aggregates consisting of C8S3 dyes of realistic parameters.



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Figure 1. 2D dispersion relations of dipolar lattices.

DOPING DEPENDENCE OF TRIONS AND OPTICAL SPECTRA IN MoS₂

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Transition metal dichalcogenide monolayers are semiconductors with a direct transition at the K-point of the Brillouin zone. The band structure of these materials has unique features that makes them ideal candidates for valleytronics. Tightly bound negative trions, a quasiparticle composed of two electrons and a hole, can be optically created with valley and spin polarized holes. They possess a large binding energy and large oscillator strength, such that they dominate optical spectra even at room temperature. Here, we solve Bethe-Salpeter equation for three particle wavefunction at finite momentum [1]. Our results enable us to explain existing data on temperature and doping dependence and predict new spectroscopic features in doped MoS₂ [1,2], as shown in Fig. 1.

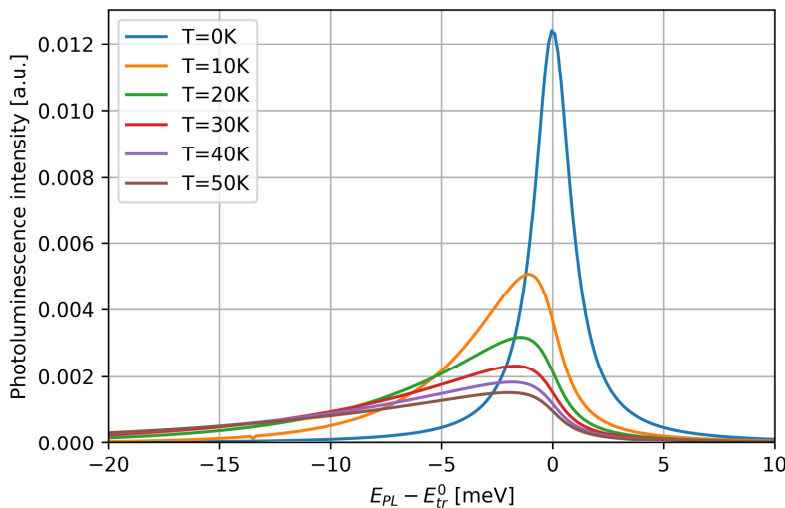


Fig.1: Temperature dependence of the calculated photoluminescence of a doped MoS₂. As the temperature increases, we find an asymmetric broadening and red shift of the emission peak.

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**CRYSTAL PHASES OF CHARGED INTERLAYER EXCITONS IN VAN DER WAALS
HETEROSTRUCTURES**

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We study the properties of charged interlayer excitons (CIE) in highly excited vdW heterostructures [1] — a compound fermion system with the permanent dipole moment observed recently in Transition-Metal-Dichalcogenide bilayer heterostructures [2]. We predict the existence of new strongly correlated collective CIE states, the long-range ordered phases of the excited heterostructure — the crystal phase and the Wigner crystal phase. We evaluate the critical temperatures and density for the formation of such many-particle cooperative compound fermion states. We demonstrate that they can be selectively realized with bilayers of properly chosen electron-hole effective mass ratio by just varying their interlayer separation distance. Compound fermion systems featuring permanent electric dipole moments are of both fundamental and practical importance due to their inherently unique many-body correlation effects between electric-dipole and spin degrees of freedom. The spin in such systems could potentially be used for quantum information processing and its correlation with the dipole moment provides an opportunity for spin manipulation through optical means. Fundamental cooperative crystallization phenomena we predict will greatly increase the potential capabilities of such systems to open up new avenues for experimental exploration and novel device technologies with van der Waals heterostructures.

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HYBRID 2D AND 3D NANOSTRUCTURED PEROVSKITES: FROM UNDERSTANDING
FUNDAMENTAL PHYSICS TO OPTOELECTRONIC APPLICATIONS

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Hybrid organic–inorganic perovskites (HOPs) have demonstrated an extraordinary potential for clean sustainable energy technologies and low-cost optoelectronic devices. This talk overviews the main features of three dimensional (3D) and layered two-dimensional (2D) HOPs by combining solid-state physics concepts with simulation tools based on density functional theory. A comparison between layered and 3D HOPs highlights differences and similarities such as spin-orbit effects, quantum and dielectric confinements and excitonic properties. In 3D HOPs we study in depth the effects of electron-phonon coupling leading to polaron formation across the broad range of materials. Calculated electronic structure, charge density, changes the geometry, and reorganization energies are further related to experimentally measured specific vibrational modes, Huang-Rhys parameters and Jahn-Teller like distortions. These effects lead to formation of meta-stable deep-level charge states, which potentially responsible for photocurrent degradation in thin-film perovskite devices. The photophysics of 2D materials is defined by an interplay of strongly bound excitons and lower-energy states associated with the edges of the perovskite layers. The latter provide a direct pathway for dissociating excitons into longer-lived free carriers that substantially improve the performance of optoelectronic devices. Our theoretical simulations rationalize specifics of electronic structure of these materials, dynamics and a role of interfacial states. We also outline specific ways to rationally control geometry of edges in 2D HOP materials via external fields, contact interfaces and composition of organic compound. Overall, our results provide insights towards the material design for various applications.

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TWO FACES OF A DOUBLE WELL: MULTIFUNCTIONAL DEVICE BASED ON A Ti_2O MONOLAYER AND MAGNETO-MECHANICAL SWITCH BASED ON A MXENE NANOTUBE

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The presentation will consist of two parts. In the first part a new concept of multifunctional nanodevices as potential replacements for common transistors will be presented and a Ti_2O monolayer as an example of such a nanodevice will be discussed. Our study based on density functional theory indicates that a Ti_2O layer is bistable for two lattice parameters, being metallic for one and semiconducting for another parameter. In a switching configuration, this provides a high current ON/OFF ratio when the layer is biased and stretched simultaneously. The high sensitivity of conductance to layer stretching can be utilized for electromechanical switching, the bistability may provide a potential for application as a nonvolatile memory bit, while the current-voltage characteristic of the material in its semiconducting phase indicates a possible use as a varistor. The second part of the presentation will be about structural and magnetic properties of MXene nanotubes. Our density functional theory-based study predicts the existence of two mutually transformable polymorphs of Mo_2C nanotubes with strikingly different properties. One polymorph exhibits unusual negative strain energy with respect to the planar Mo_2C structure and the absence of any long-range magnetic order. The second polymorph displays an antiskyrmionic spin texture with a net magnetization along the tube's axis. The two nanotube polymorphs may be converted into each other by axial tensile or compressive strains, allowing for their application as a magneto-mechanical switch and eventually a nonvolatile magnetic memory unit.

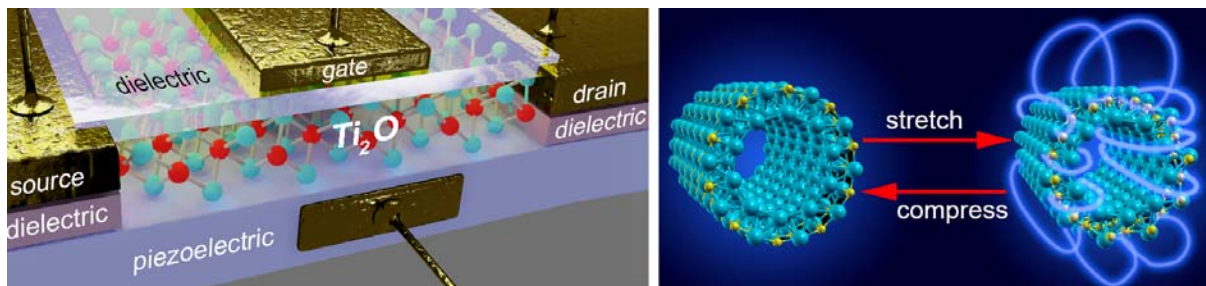


Figure 1. Bistable nanodevices based on layered Ti_2O and MXene nanotubes

STRONG LIGHT-MATTER COUPLING IN 2D ATOMIC CRYSTALS

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Two-dimensional (2D) van der Waals materials have emerged as a very attractive class of optoelectronic material due to the unprecedented strength in its interaction with light. In this talk I will first discuss the formation of exciton-polaritons [1] and their spin-optic control [2] in the 2D transition metal dichalcogenide (TMD) systems. Following this, I will discuss the formation of polaritons using excited states (Rydberg states) to enhance the nonlinear polariton interaction [3]. Recent results on electrical control and realization of a polariton LED based on 2D TMDs [4] will also be presented.

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PHASE TRANSITIONS AND EXCITON SUPERFLUIDITY IN DOUBLE LAYERS OF NOVEL
TWO-DIMENSIONAL NANOMATERIALS

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This talk reviews the theoretical studies of the Bose-Einstein condensation (BEC) and superfluidity of indirect excitons in quasi-two-dimensional (quasi-2D) van der Waals nanomaterials such as transition metal dichalcogenide (TMDC) heterostructures and phosphorene. Indirect excitons are the Coulomb-bound pairs of electrons and holes confined to different parallel monolayers of a layered planar nanomaterial structure. The high-T superfluidity of the two-component weakly-interacting Bose gas of the A-type and B-type indirect excitons in the TMDC heterostructures is proposed [1,2]. The critical temperature and superfluid velocity of the indirect excitons in a bilayer phosphorene nanostructure is shown to be anisotropic, dependent strongly on the particular direction of the exciton propagation [3]. We propose to control of electron-hole superfluidity in semiconductor coupled quantum wells and double layers of 2D material by an external periodic potential [4]. The latter can either be created by periodic gates attached to quantum wells or the double layers of 2D material or by the Moiré pattern of two twisted layers. Treating the electron-hole pairing within the mean-field approach, we apply the tight-binding approximation of the single electron spectrum and study the effect of the additional periodic potential on the electron-hole plasma-superfluid transition. The electron-hole pairing order parameter as a function of the temperature, the charge carrier density, and the gate parameters are obtained by minimization of the mean-field free energy. The second order phase transition between superfluid and electron-hole plasma, controlled by the external periodic potential, is studied for various parameters.

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**BERRY PHASES IN THE MOIRÉ PATTERNS OF TWISTED TMD BILAYERS WITH
UNIFORM AND NON-UNIFORM STRAINS**

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Long wavelength moiré pattern in van der Waals stacked 2D materials has provided a powerful tool towards designer quantum materials that can extend the exotic properties of the building blocks. For band edge carriers located at the Brillouin zone corners (valleys), the interlayer coupling features sensitive dependence on the atomic registry between the constituting layers. In twisted TMDs homobilayers, such coupling in the moiré pattern manifests itself as a location-dependent Zeeman field acting on the active layer pseudospin, which exhibits a spatial texture that gives rise to non-Abelian Berry connections. We show that Abelian Berry phase in the adiabatic limit and geometric scalar correction together realizes fluxed superlattices tunable by twist angle, strain and interlayer bias, underlying the quantum spin Hall effect discovered in low energy mini-bands [1,2]. We will also discuss carrier dynamics in moiré patterns distorted by non-uniform strains, and show how the interplay of moiré interlayer coupling and strain together leads to non-Abelian Berry phase effects [3].

The work was supported by Research Grant Council of HKSAR (17302617, 17312916, C7036-17W).

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International Workshop on Nanotechnology (Tnano20)
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**STRONGLY CORRELATED PHASES OF MATTER IN SEMICONDUCTOR
MOIRÉ SUPERLATTICES**

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Moiré superlattices built on monolayer transition metal dichalcogenide (TMD) semiconductors have presented a unique platform to explore the physics of a single-band Hubbard model. In this talk, I will discuss the emergence of Mott insulating states, charge-ordered states, stripe phases and electronic liquid crystal states in this strongly correlated system.

DEFECTS AND DEFECT DYNAMICS IN NOVEL 2D MATERIALS

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Exciting the evolution of defects and simultaneously imaging the dynamical process can be realized with an aberration corrected electron beam inside the ultrahigh vacuum scanning transmission electron microscope (STEM). This method offers time-resolved direct tracking of the atomic motion during the structural changes induced by the high energy electrons. By controlling the scanning pattern of the electron beam, manipulation of defect to create new nanostructures is achievable. I will first show the atomic scale characterizations of defect structures in various emerging 2D materials by low-voltage STEM, including monolayer amorphous carbon, air-sensitive NbSe₂ monolayer and 1T' phase Te-based alloy monolayer, and elaborate how they affect the physical properties of the materials by combining density functional theory (DFT) calculations. Then I will demonstrate the atom-by-atom structural evolutions in 2D materials as monitored by sequential low voltage Z-contrast STEM imaging and the related underlying physics. Examples include Se vacancy-induced inversion domain nucleation in MoSe₂, the origin of novel 2D Pd₂Se₃ phase driven by interlayer fusion in layered PdSe₂, and the in situ observation of electron beam induced synthesis of hexagonal MoSe₂ from square FeSe. At the end of the talk, I will discuss the in-situ fabrication of highly stable metallic nanowires with MX stoichiometry within the transition-metal dichalcogenide (TMD) monolayers by steering the electron beam with atomic precision.

INDUCED SUPERCONDUCTIVITY IN THE FRACTIONAL QUANTUM HALL EDGE IN
GRAPHENE HETEROSTRUCTURES

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Topological superconductors represent a phase of matter whose properties cannot be smoothly changed from one phase to another, a robustness which renders them suitable for quantum computing. The past decade has witnessed substantial progress towards a qubit based on Majorana modes, non-Abelian excitations whose exchange—braiding—produces topologically protected logic operations. However, because braiding Majoranas cannot provide a universal quantum gate set, Majorana qubits are computationally limited. This drawback can be overcome by parafermions, a novel set of non-Abelian modes whose array supports universal topological quantum computation. The primary route to synthesize parafermions involves inducing superconductivity in the fractional quantum Hall (fqH) edge. In this presentation we use high-quality van der Waals devices, coupled to narrow superconducting NbN, in which superconductivity and robust fqH coexist. We find crossed Andreev reflection (CAR) across the superconductor separating two counterpropagating fqH edges which demonstrates their superconducting pairing. The CAR probability of the integer edges is insensitive to magnetic field, temperature, or filling, providing evidence for spin-orbit coupling which enables the pairing of the otherwise spin-polarized edges. FqH edges, however, may show a higher CAR probability varying with temperature, an observation contrasting with that in integer edges. Control experiments show that CAR vanishes at high temperature and excitation as expected from the finite superconducting and fqH energy gaps. These results demonstrate all the required ingredients for parafermions, laying the groundwork for their experimental research in condensed matter.

2D AND TOPOLOGICAL MAGNETIC MATERIALS

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Two dimensional (2D) magnets and heterostructures with topological insulators (TI) present new opportunities for energy-efficient spintronic devices due to their low magnetic volume, high spin-torque efficiency, novel quantum states, and interfacial proximity effects. Our focus is to develop robust room temperature 2D magnets, to understand the electronic, chemical, and magnetic interactions at 2D magnet-TI interfaces, and to realize spintronic functionality and novel magnetic topological states. Here, we describe our work utilizing molecular beam epitaxy for precise, atom-by-atom deposition of van der Waals materials consisting of MnSe₂, Bi₂Se₃, and MnBi₂Se₄. Starting with the epitaxial growth of MnSe₂ on GaSe and SnSe₂ base layers, we observed room temperature ferromagnetism in the monolayer limit [1]. Subsequent integration of MnSe₂ onto the topological insulator Bi₂Se₃ revealed chemical migration and dipole formation at the interface [2]. Specifically, we learned of the propensity for the MnSe₂ to intermix with the underlying Bi₂Se₃ to form a MnBi₂Se₄ septuple layer. By repeating the deposition of a Bi₂Se₃ followed by MnSe₂, we synthesized multilayer MnBi₂Se₄ for the first time (Figure 1a) [3]. This material is the cousin of the well-studied MnBi₂Te₄, a magnetic topological insulator exhibiting quantum anomalous Hall effect and axion insulator state. Angle-resolved photoemission spectroscopy of our MnBi₂Se₄ shows the presence of a topological Dirac surface state (Figure 1b). Magnetic measurements provide evidence of a layered antiferromagnetic state, similar to that observed in MnBi₂Te₄, but with an in-plane orientation of the magnetic moments which could give rise to alternative topological states.

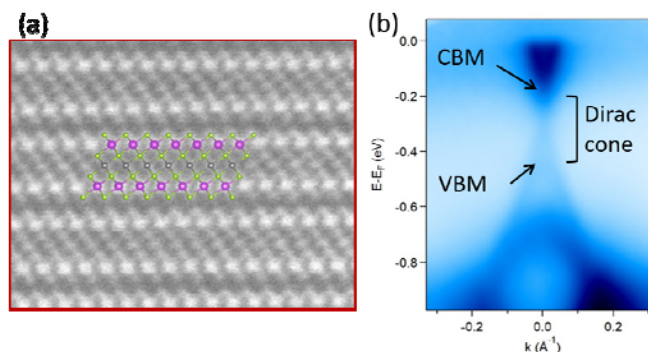


Figure 1. (a) TEM image of MnBi₂Se₄. (b) ARPES showing topological Dirac surface state.

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BCS-BEC CROSSOVER IN A 2D SUPERCONDUCTOR

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Gate-induced superconductivity using field effect transistor devices has a strong advantage over the conventional bulk superconductivity owing to its controllability. To realize the gate-induced superconductivity, researchers have nowadays established two methods; one is to use gate dielectrics which enables high density carrier accumulation, which is sufficient to achieve superconductivity in semiconductors. The other is to use channel materials with huge lattice parameters, which enable the effective high band-filling with a rather low carrier density. The former was realized by ionic gating first on SrTiO₃ followed by many 2D materials [1]. The latter was achieved in 2018 [2] on magic angle twisted bilayer graphene.

In this presentation, we focus on the ion-gated superconductors and report our challenge to approach the Bose-Einstein condensation (BEC) region, where preformed pairs are formed at high temperatures and condense at lower temperature. BEC in superconductivity is believed to be realized in the low carrier density limit. However, most of superconductivity is realized in high carrier densities and classified as the Bardeen-Cooper-Schrieffer (BCS) condensation, in which the condensation and pairing occurs simultaneously. The crossover from BCS to BEC has been a long-time challenge in materials science of superconductors.

By controlling the gating protocol in Li intercalated layered compound, Li_xZrNCl, we have succeeded in controlling x from 0.28 to 0.004, and established the phase diagram by simultaneous experiments of resistivity and tunneling spectra under the ionic gating. T_c exhibits dome-like behavior, and more importantly, a wide pseudogap phase was discovered in the low doping regime. Furthermore, in the low carrier density limit, T_c scales as $T_c/T_F = 0.12$, where T_F is the Fermi temperature, which shows fair agreement with the theoretical prediction in the 2D limit of BEC [3].

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PAIRING TRANSITION IN INTERACTING ELECTRONIC DOUBLE LAYERS

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In a system of two parallel two-dimensional layers we study the pairing transition caused by interlayer Coulomb interaction. Depending on the charge carriers, which can be electrons or holes, the interaction is either repulsive for two electron layers or attractive for an electron and a hole layer. In the latter case the paired state consists of excitons [1] while in the former case we get electron pairs [2]. It is important that these two pairing states are related by a duality transformation. The pairing transition depends on the density of states and requires a critical interaction strength in the case of a honeycomb lattice, where the density of states vanishes at the Fermi energy (Figure 1 left). The paired states have a characteristic behavior in terms of the optical conductivity, which reflects the Coulomb drag effect (Figure 1 right).

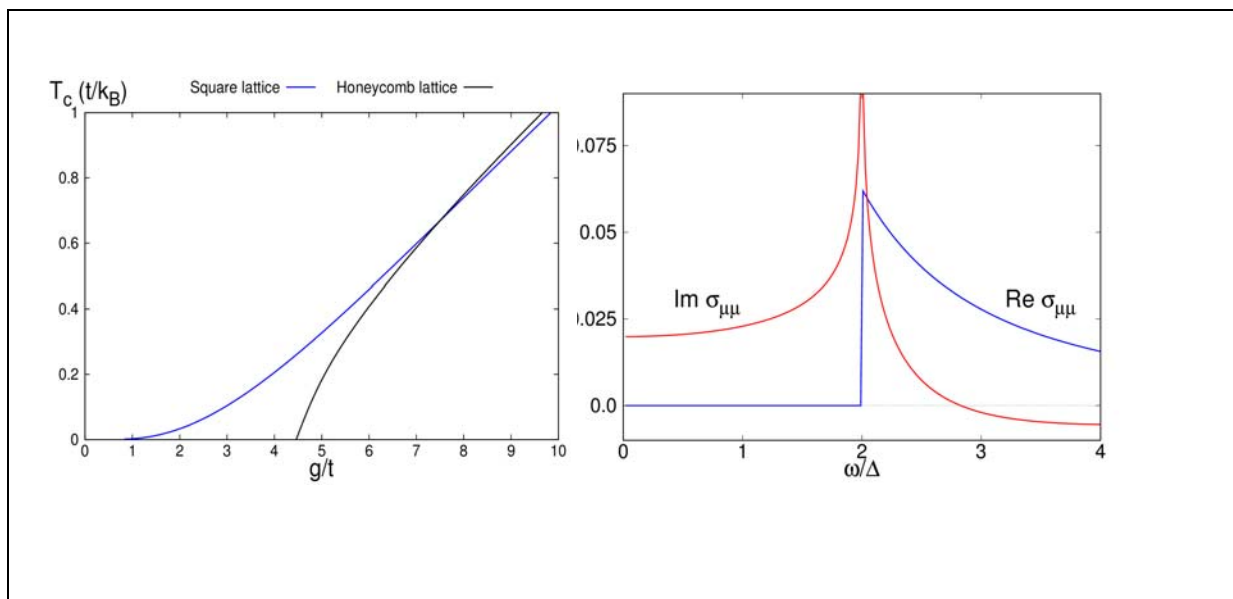


Figure 1. Left panel: critical temperatures for a square lattice and a honeycomb lattice as a function of the interaction strength g . Right panel: Optical conductivity of frequency ω describes the Coulomb drag.

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ELECTROSTATIC COOLING AT ELECTROLYTE-ELECTROLYTE JUNCTIONS

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Heat effects are of great importance in nanotechnology and electrochemical engineering and other fields. Electrostatic heating and cooling is observed when current is driven through an electrical double layer (EDL), i.e., the structure formed at the interface of two oppositely charged materials. Dependent on current direction, there is either cooling or heating. This is exactly what happens in a Peltier element at the interface of two solid, electron-conducting phases. The same also happens at the water-metal interface, e.g., in microporous carbon electrodes. Here we report heating and cooling at a water-water interface between two electrolyte phases. These phases are water + salt, and an ion-exchange membrane. Such a membrane is a highly charged (5 M of fixed charges !) microporous structure filled with water and ions. We discuss the theory and experimental validation of reversible heating and cooling at electrolyte-electrolyte junctions. Key to the theory is identification that the heating and cooling is described by the dot product of the vectors current and field strength, which can be both positive and negative, and not by Joule heating, an approximation only valid under strict assumptions, and which is strictly positive, and cannot explain electrostatic cooling.

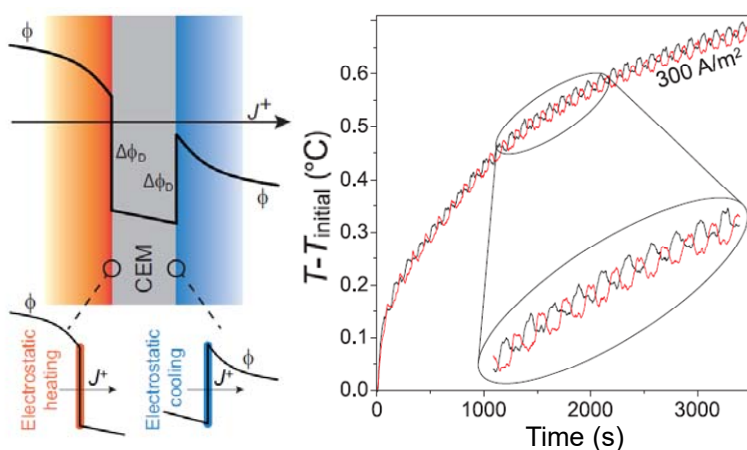


Figure 1. (Left) Heating and cooling at the junctions between two aqueous phases, in this case at the two outsides of a cation-exchange membrane (CEM), which is a charged, water-filled, microporous structure. (Right) Heat production at each membrane interface (red and black curves) fluctuates between heating and cooling upon changing the direction of current.

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ALL YOU WANTED TO KNOW ABOUT PUBLISHING IN PHYSICAL REVIEW JOURNALS

Athanasios CHANTIS

PHYSICAL REVIEW Journals, Ridge, New York, NY, USA

The track record and commitment of PHYSICAL REVIEW journals to high quality, scientific honesty and fairness, and coverage of the entire field of Physics is unprecedented. This also applies to the rapidly evolving field of Nanotechnology, the topic of this workshop. Many presenting authors at this workshop are aware of innovative ways undertaken by PHYSICAL REVIEW to attract cutting-edge, high quality research in 2D materials and devices by dedicating a collection of invited contributions to this topic [1].

This presentation will provide information about the publishing process in PHYSICAL REVIEW journals. An Editor will introduce the spectrum of PHYSICAL REVIEW journals and will give a brief overview of the peer review process in PHYSICAL REVIEW. The current and future status of scientific publishing will be discussed. This presentation will be followed by an open floor discussion with editors from Phys. Rev. Letters, Phys. Rev. X, Phys. Rev. B, Phys. Rev. Applied, and Phys. Rev. Materials.

References

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<https://journals.aps.org/prapplied/collections/two-dimensional-materials>,
<https://journals.aps.org/prmaterials/collections/two-dimensional-materials>

DEFECTS AND THEIR INFLUENCE ON THE THERMOELECTRIC PROPERTIES OF
MATERIALS: AN *AB INITIO* STUDY

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For thermoelectric applications, *ab initio* methods generally fail to predict the transport properties of materials because of their inability to predict properly the carrier concentrations that control the electronic properties. Concerning the thermal properties, the study of the impact of defects is mainly hindered by the huge computer resources needed to consider the large supercells necessary for this kind of study.

In this presentation, a methodology based on the thermodynamics of defects and the phase stability supposed to fill in this gap (especially concerning the electronic properties) is presented. It is then applied to several thermoelectric materials belonging to the Heusler family. We show for the NiTiSn [1] half-Heusler compound that by taking into account the scattering of phonons by the grain size boundaries (*i.e.* nanostructuring), a good agreement of the calculated thermal conductivity with experiments can be obtained. Similarly in the Fe₂VAl Heusler compound [2], the existence of cubic Al-V antiphase clusters around an Iron atom permits to explain the peculiar measured electronic properties of this material.

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SCATTERING OF PLASMONS IN CLOSELY PACKED 1D GRAPHENE STRUCTURES

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We present a comprehensive study of graphene plasmon eigenmodes in 1D periodic structures formed by plasmonic junctions of different types. Transmission and reflection coefficients composing scattering matrix of a junction are obtained directly from numerical solutions of equations describing the plasmons in the considered structures. The obtained results for the single junctions are in perfect agreement with analytical formulas for the cases when they are available. Using our method as a reference, we analyze the limitations of the semi-phenomenological transfer matrix approach applied to the calculation of reflection from the double-junction structures. Our results can be useful in designing and calculating graphene plasmon resonators, waveguides, switches, etc.

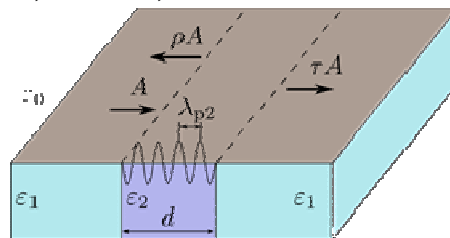


Figure 1. Schematic view of the graphene plasmon double-junction supported by a wafer with discontinuously changed dielectric permittivity.

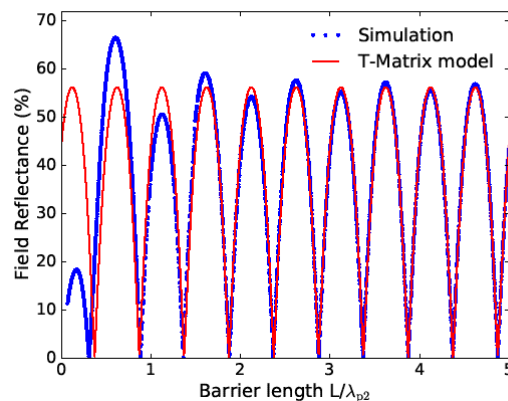


Figure 2. Absolute value of the reflection coefficient of a plasmon in graphene scattered on a barrier formed by the two junctions versus its normalized length. Solid line shows the reflectance predicted by a transfer matrix model, and circles are calculated with our numerical analysis.

NEW PHOSPHORUS STRUCTURES:
FROM TYPE-II RED PHOSPHORUS TO PHOSPHORENE EDGES

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Various allotropes and polymorphs of phosphorus have gained wide attention. In the first part of my talk, I will discuss our effort to identify the crystal structure of type-II red phosphorus (RP), which has not been solved for the last 70 years [1]. RP, an allotrope of phosphorus which is usually known to be amorphous, has several types of crystalline phases. The crystal structures of type-IV (fibrous RP) and type-V (Hittorf 's phosphorus) have been previously identified by single-crystal X-ray crystallography, however, those of type-II and type-III phases are yet to be identified. We identified the crystal structure of type-II RP using complementary characterization with power X-ray diffraction, 3D electron diffraction, and atomic-resolution scanning transmission electron microscopy (STEM) [2], as seen in Fig. 1. We confirmed that type-II RP has a large triclinic unit cell with approximately 500 phosphorus atoms. Moreover, STEM images clearly revealed the local tubular structure of phosphorus. In the second part of my talk, I will present on the modification of black phosphorus (BP) edges [3] using in situ heating under TEM imaging. We observed the formation of ultra-high stability zigzag phosphorene edges at elevated temperatures [4]. From the edge structure investigation, we found that the phosphorus atoms at edges are merged together to form closed zigzag phosphorene edges. We envision that these newly identified phosphorus structures facilitate various fundamental studies on phosphorus allotropes and polymorphs.

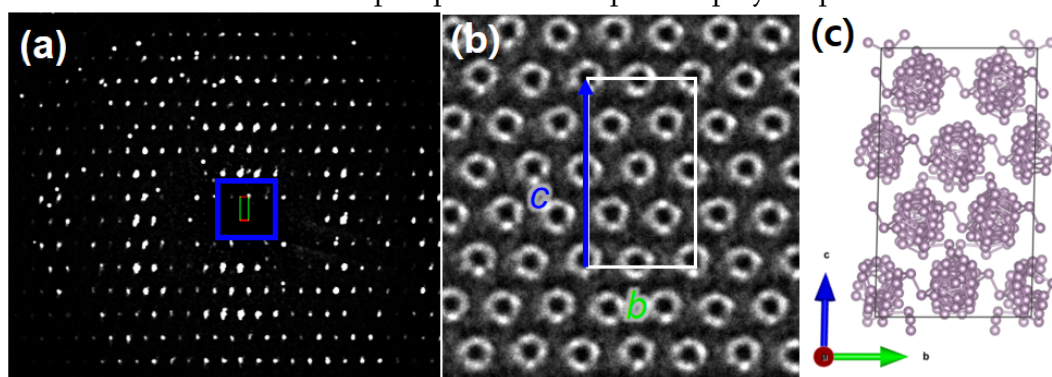


Figure 1. Structure characterization of type-II red phosphorus. (a) 3D electron diffraction, (b) Cross-sectional STEM image, (c) Atomic model of type-II red phosphorus

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VIOLET PHOSPHORUS AND PHOSPHORENE

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Black phosphorene has attracted much attention as a semiconducting two - dimensional material. Violet phosphorus is another layered semiconducting phosphorus allotrope with unique electronic and optoelectronic properties. However, no confirmed violet crystals or reliable lattice structure of violet phosphorus had been obtained. Now, violet phosphorus single crystals were produced and the lattice structure has been obtained by single - crystal x - ray diffraction to be monoclinic with space group of $P2/n$ (13) ($a=9.210 \text{ \AA}$, $b=9.128 \text{ \AA}$, $c=21.893 \text{ \AA}$, $\beta=97.776^\circ$). The lattice structure obtained was confirmed to be reliable and stable. The optical band gap of violet phosphorus is around 1.7 eV, which is slightly larger than the calculated value. The thermal decomposition temperature was 52 °C higher than its black phosphorus counterpart, which was assumed to be the most stable form. Violet phosphorene was easily obtained by both mechanical and solution exfoliation under ambient conditions.

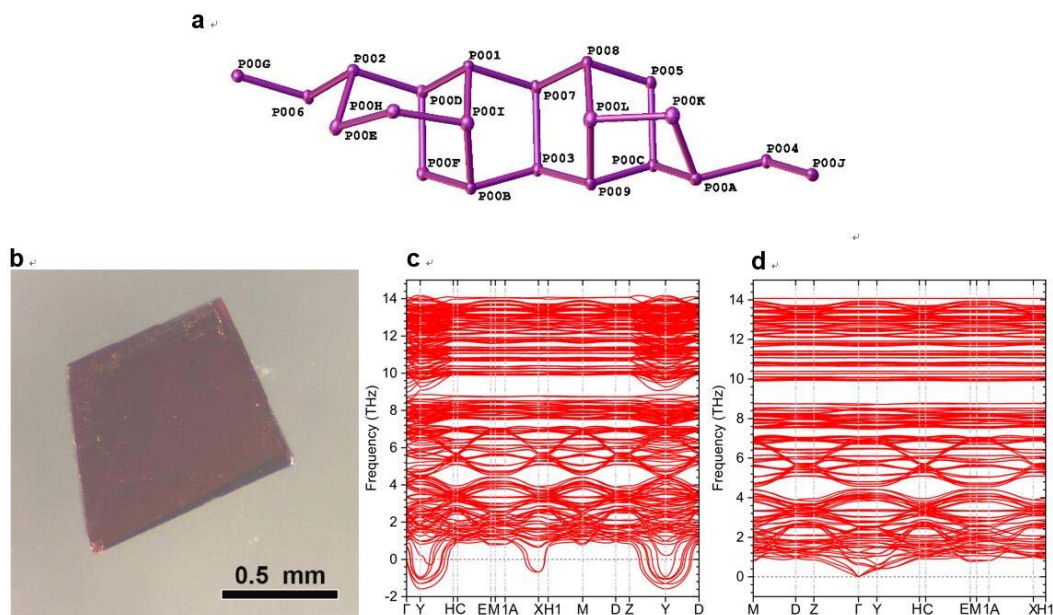


Figure 1. The crystal structure of violet phosphorus. (a) Minimum asymmetric unit; (b) Optical microscope image of a violet phosphorus single crystal; The phonon dispersive curves of violet phosphorus (c) from 1969 and (d) our violet phosphorus in the Brillouin zone.

DOUBLE RESONANT RAMAN SCATTERING IN TMDCs

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Raman spectra of TMDCs have been reported for several decades. The first-order Raman process in TMDCs has been widely investigated and is now well understood. However, the study of second-order Raman spectra did not yet give consistent assignments for different TMDCs. We study the second-order Raman process of monolayer TMDCs, by combining *ab initio* density functional perturbation calculations with experimental Raman spectroscopy and electron-phonon Wannier (EPW) method [1-4]. The calculated electronic band structure and the density of states show that the resonance Raman process occurs at the M point in the Brillouin zone (**Figure 1**), where a strong optical absorption occurs due to a logarithmic Van Hove singularity of the electronic density of states. The double resonance Raman process with intervalley electron-phonon coupling connects two of the three inequivalent M points in the Brillouin zone, giving rise to second-order Raman peaks due to the M-point phonons. The calculated vibrational frequencies and laser-energy dependent Raman spectra of the second-order Raman spectra agree with the observed laser-energy-dependent Raman shifts in the experiment. We also predicted the helicity dependence of the double resonant Raman modes.

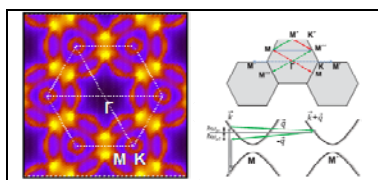


Figure 1. (left) Optical absorption in the Brillouin zone at a certain laser energy. (right) The schematics of the double resonance process (electron-photon and electron-phonon processes).

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LOW-SYMMETRY TWO-DIMENSIONAL STRUCTURES WITH
ANISOTROPIC HIGH CARRIER MOBILITY

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A strong in-plane anisotropy of carrier transportation was found in black phosphorene [1], which provides another degree of freedom for tuning the physical properties of 2D materials and thus expands the range of opportunities for designing novel 2D semiconductors with unique applications. By combine graphene and black phosphorene, a series of previously unknown allotropes of phosphorus carbide (PC) in the stable shape of an atomically thin layer have been predicted [2]. As a result of the competition between sp^2 bonding found in graphitic C and sp^3 bonding found in black P, the PC structures can display as semi-metals with an anisotropic Dirac cone, or narrow-gap semiconductors with a strong anisotropic high carrier mobility. The relatively narrow band gaps of semiconducting PC structures can be further tuned by the approach of isoelectronic substitution. Previous unknown novel low-symmetry 2D ternary 2D structures have been designed. Sharing the geometry of 2D PC, the predicted 2D ternary structures display a strong in-plane anisotropy together with band gaps covering a wider range and broader the potential of applications in the novel nano-devices.

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QUANTUM DEVICES WITH 2D SEMICONDUCTORS AND INSULATORS

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In this talk I will describe two applications of 2D layered materials for quantum devices. First, I will discuss our work to fabricate and characterize gate-defined, accumulation mode quantum dots using monolayer and bilayer WSe₂ (**Figure 1**) [1]. The devices are operated with gates above and below the WSe₂ layer to accumulate a hole gas, which for some devices is then selectively depleted to define the dot. Temperature dependence of conductance in the Coulomb-blockade regime is consistent with transport through a single level, and excited-state transport through the dots is observed at temperatures up to 10 K. These devices provide a platform to evaluate valley-spin states in monolayer and bilayer WSe₂ for application as qubits. Second, I will discuss gate-tunable Josephson junction field-effect transistors (JJ-FETs) based on Al/InAs in which the gate dielectric is thin hBN [2]. Comparing devices with hBN and AlO_x dielectrics, we observe that the product of normal resistance and critical current, $I_c R_n$, is comparable for both types of devices, but strikingly higher R_n for the hBN-based devices indicating that the surface is doped less compared to AlO_x gate dielectric. These results demonstrate that h-BN provides a superior gate dielectric compared to AlO_x for JJ-FET devices with applications in superconducting logic and quantum information technologies such as gatemon qubits and topological superconductivity.

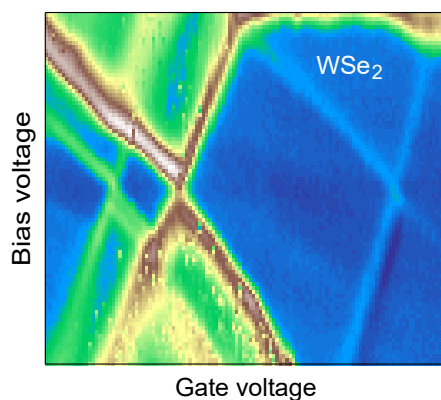


Figure 1. Coulomb diamond with resolved excited states for a gate-defined bilayer WSe₂ quantum dot.

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2D VAN DER WAALS HETEROSTRUCTURES FOR EMERGING DEVICE APPLICATIONS

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Van der Waals (vdW) heterostructures are formed by stacking layers of different 2D materials and offer the possibilities to design new structures with atomic-level precision. In this talk, I will show how these heterostructures provide unprecedented opportunities to realize emerging device applications, especially in the fields of memory, computing and advanced optoelectronics.

I will first show that robust memristors with good thermal stability, which is lacking in traditional memristors, can be created from a vdW heterostructure composed of graphene/MoS_{2-x}O_x/graphene. The devices exhibit excellent memory performance with an endurance of up to 10⁷ and a high operating temperature of up to 340 °C. With the help of *in situ* electron microscopy, we revealed the origin of good thermal stability and a possible switching mechanism.[1] We also observed ballistic avalanche phenomena in a thin vdW heterostructure made of black phosphorus and Indium Selenide (InSe). Such phenomena can be utilized to realize efficient carrier manipulation and develop advanced optoelectronic devices. [2] Our latest results on a gate-tunable vdW heterostructure for reconfigurable neural network vision sensor, as well as an electrically tunable homojunction for reconfigurable logic and neuromorphic circuits will also be presented. [3, 4]

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GATE TUNABLE ANISOTROPY IN 2D GATE

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Anisotropy in crystals arises from different lattice periodicity along different crystallographic directions, and is usually more pronounced in two dimensional (2D) materials. Indeed, in the emerging 2D materials, optical and electrical anisotropy has been one of the recent research focuses [1]. However, key understandings of the in-plane anisotropic resistance in low-symmetry 2D materials, as well as demonstrations of model devices taking advantage of it, have proven difficult. Here, we show that, in few-layered semiconducting GaTe, electrical conductivity anisotropy between x and y directions of the 2D crystal can be gate tuned from several fold to over 10^3 [2]. This effect is further demonstrated to yield an anisotropic non-volatile memory behavior in ultra-thin GaTe, when equipped with an architecture of van der Waals floating gate (Figure 1).

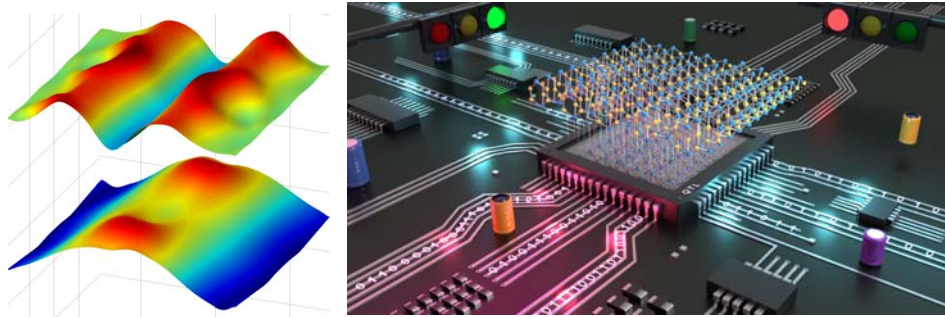


Figure 1. (left) Band profile of top valence and bottom conduction bands; (right) anisotropic non-volatile “traffic control” memory.

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DEVICE APPLICATIONS OF MXENES

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MXenes are members of a new 2D material family of metal carbides and nitrides that could be utilized in nanoscale devices. We have investigated three types of MXene-based nanodevices. First, we have calculated the device characteristics of a magnetic tunnel junction (MTJ). Half-metallic Mn_2CF_2 MXene layer was selected as the magnetic electrode, and structurally compatible Ti_2CO_2 as the transport barrier, as shown in Figure 1. We find that the tunneling magnetoresistance ratio has a peak value of 10^6 . Second, we have considered a $\text{Mo}_2\text{TiC}_2\text{O}_2$ -based quantum transport device as a pressure sensor. In a compressed double MXene, the electronic states originating from the two different transition metals are shifted up unequally. Thus, the character of the valence band maximum (VBM) changes drastically after a critical compression. The proposed nanodevice has moderate pressure sensitivity. While the macroscopic $\text{Mo}_2\text{TiC}_2\text{O}_2$ sensor is usable only for excess pressure detection, the nanodevice can act as a pressure sensor in a wider pressure range. The same mechanism of pressure-induced unequal level-shifting could be exploited also in other double MXenes.

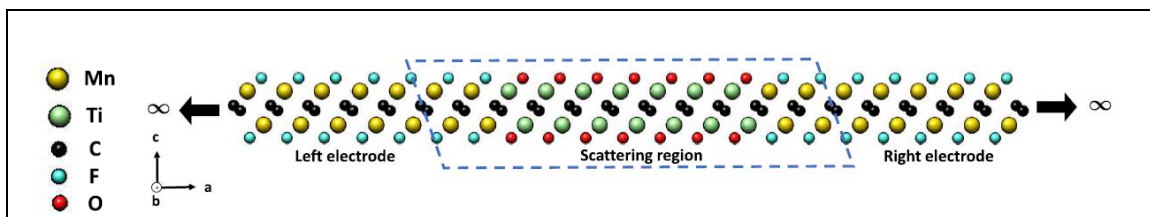


Figure 1. MXene-based MTJ device model.

Third, we propose an MXene-based field-effect transistor, consisting of semiconducting Ti_2CO_2 seamlessly connected to metallic Ti_2CF_2 electrodes of the same family. Our non-equilibrium Green's function (NEGF) quantum transport calculations reveal that the smallest feature size is approximately 6 nm for the gate-controlled current. Changing the surface termination alters the electronic states to allow gate-controlled currents. The positive gate voltages increase the current, while the negative values have the opposite effect. As the surface terminations of the electrodes are not crucial, modification of the termination only in the scattering region is sufficient. The ultrathin Ti_2CT_2 MXene-based nanodevices are thus feasible candidates for efficient field-effect transistors.

Given the excellent stability of MXenes, they are promising ingredients for nanoscale device applications.

TUNABLE SPIN-ORBIT COUPLING IN A HIGH MOBILITY FEW-LAYER SEMICONDUCTOR

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In a crystal, the two-fold degeneracy of spins is protected by the combined inversion symmetry in both space and time. In the well-known Zeeman effect, an external magnetic field breaks the time reversal symmetry (TRS) and splits the spin degeneracy by $g\mu_B B$, where g is the gyromagnetic ratio and μ_B is Bohr magneton. Alternatively, the spin degeneracy can be lifted by spin-orbit coupling (SOC) when spatial inversion symmetry is broken, even in the absence of a TRS-breaking magnetic field, leading to a variety of magnetic, spintronic and topological phases and applications. In conventional bulk materials, the SOC parameter is a constant that cannot be modified. Here we exploit the tunability of two-dimensional (2D) materials, and demonstrate SOC and zero-field spin-splitting in atomically thin InSe that can be modified over an unprecedentedly large range. From beating patterns in quantum oscillations, we establish that the SOC parameter α is thickness-dependent; it can be continuously modulated over a large range by an out-of-plane electric field, achieving zero-field splitting tunable between 0 and 20 meV. Surprisingly, α could be enhanced by an order of magnitude in some devices, suggesting that SOC can be further manipulated by variations in interlayer spacing induced by stacking and/or electrostatic compression. Our work highlights the extraordinary tunability of SOC in 2D materials, which can be harnessed for *in operando* spintronic and topological devices and applications.

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UNUSUALLY STRONG “HIDDEN” RASHBA EFFECTS IN Si₂Bi₂

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In addition to spin-orbit coupling (SOC), it is an asymmetric crystal potential that induces Rashba (R-1) spin splitting observed at surfaces or interfaces. The R-1 states are characterized by a Mexican hat-like band dispersion with spin-momentum locking described by

$$H_R = -\alpha_R \boldsymbol{\sigma} \times \mathbf{k} \cdot \hat{z},$$

where α_R , $\boldsymbol{\sigma}$, and \mathbf{k} are Rashba strength coefficient, Pauli spin matrix, and crystal momentum; and \hat{z} indicates the direction of local electric field created by the asymmetric crystal potential. Recently, it has, however, been found that even centrosymmetric materials can exhibit a similar but distinct spin splitting called “hidden” Rashba (R-2) effect, such as spatially-segregated spin splitting or spin-layer locking (SLL) as shown in Fig. 1. To understand the underlying physical origin of such R-2 phenomena, we used the first-principles density functional theory and model Hamiltonian calculation to investigate a new two-dimensional (2D) materials Si₂Bi₂, which we identified to possess an ideal condition for the strong R-2 SLL. Our study revealed that the hidden SLL can be determined by a competition between the SOC and sublayer-sublayer interaction. We evaluated the Rashba strength to be 2.16 eVÅ, which is the greatest value ever observed in 2D R-2 material to the best of our knowledge. [1, 2]

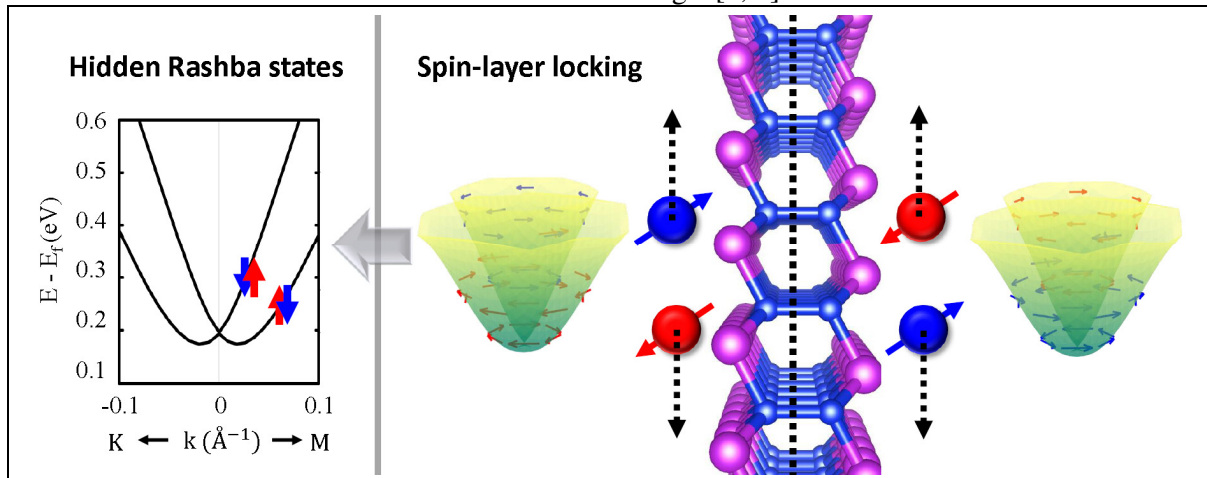


Figure 1. Hidden Rashba states corresponding to the spatially segregated Rashba spin splitting called spin-layer locking observed in an equilibrium phase of Si₂Bi₂ with the inversion symmetry.

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CELL POLARITON: A QUANTUM STATE IN THE MYELIN SHEATH OF A NERVE

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Various polaritons are raising significant interest in physics and materials science for their unique and unexpected properties, especially their condensation, lasing without population inversion, and even room-temperature superfluidity. Here, we propose a cell polariton (CP): a collective coherent mode of a photon with the ensemble of all phospholipid molecules in a myelin sheath formed by glial cells. CP can be found resonantly self-confined in the myelin sheath under physiological conditions. This mode arises from the very compact, ordered and polar thin-film structure of the sheath, and the relatively strong coupling between the mid-infrared photon and the vibration modes of phospholipid tails in the myelin. The collective CP mode is then basically a coherent superposition of the photon and vibration modes within the myelin. It enhances the myelin permittivity significantly and forms a resonance state that involves the sheath cell. Our findings provide a new understanding of highly efficient energy utilization by neural cells, as well as a paradigm for the design of highly efficient energy transport in materials and devices.

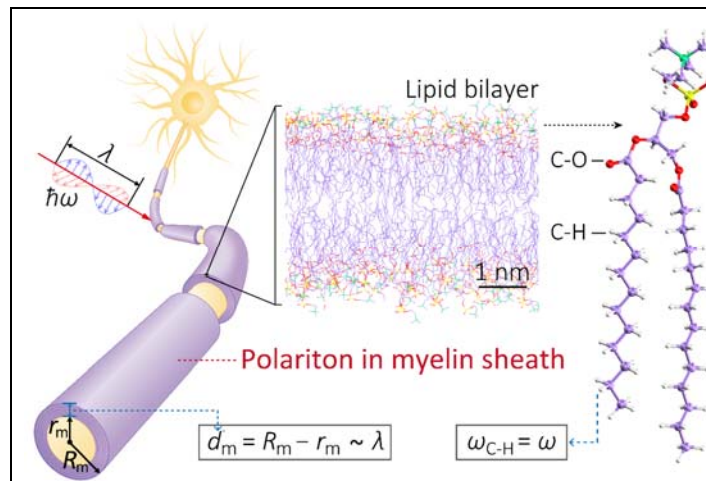


Figure 1. Cell-polariton resonantly and coherently forming in myelin sheath.

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SEMICONDUCTING LAYERED TRANSITION-METAL DICHALCOGENIDES:
INSIGHTS FROM FIRST-PRINCIPLES

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Transition-metal dichalcogenides (TMDCs) are an important class of inorganic materials exhibiting a wide spectrum of catalytic, electronic, magnetic, and optical properties [1]. In particular, TMDCs with layered structures such as MoS₂ are considered attractive for use in next-generation nanoscale flexible field-effect transistor (FETs) devices [2] and for the important areas of industrial heterogeneous catalysis [3]. TMDCs nanomaterials (i.e., nanotubes and fullerene- or onion-like structures) have also emerged as possible applications as photodetectors or photo electrochemical solar cells [4].

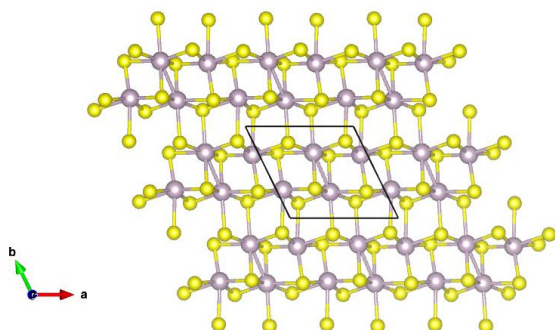


Figure 1. Ball-and-stick model of the layered TcX₂ (X=S and Se). Top view along the normal to the (a,b) plane. Color legend: Tc, blue; X, yellow.

Among TMDCs, relatively limited knowledge is available on technetium dichalcogenides (Figure 1). A systematic study of the structures and properties of layered technetium dichalcogenides investigated using density functional theory (DFT) [5] indicates that they are semiconducting. Structure-property relationships of this fascinating tunable bandgap materials will be discussed in this talk.

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Alphabetic List of Contributors, Affiliations and Abstracts

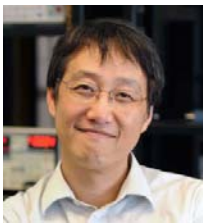
Keynote Lectures (listed by alphabet)



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MAGIC-ANGLE GRAPHENE: CORRELATIONS,
SUPERCONDUCTIVITY, AND BEYOND



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INDUCED SUPERCONDUCTIVITY
IN THE FRACTIONAL
QUANTUM HALL EDGE IN
GRAPHENE HETEROSTRUCTURES

Invited Lectures (listed by alphabet)

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DEVICE APPLICATIONS OF MXENES

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PHASE TRANSITIONS AND EXCITON SUPERFLUIDITY IN DOUBLE
LAYERS OF NOVEL TWO-DIMENSIONAL NANOMATERIALS

Maarten BIESHEUVEL

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Sustainable Water Technology,
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ELECTROSTATIC COOLING AT ELECTROLYTE-ELECTROLYTE
JUNCTIONS

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CRYSTAL PHASES OF CHARGED INTERLAYER EXCITONS IN VAN
DER WAALS HETEROSTRUCTURES

Athanasios CHANTIS

Physical Review
Ridge, NY, USA

ALL YOU WANTED TO KNOW ABOUT PUBLISHING IN PHYSICAL
REVIEW JOURNALS

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UNIVERSAL SCALING OF THE ANISOTROPIC DISPERSION IN 2D
EXCITONIC SYSTEMS AND ITS SPECTROSCOPIC SIGNATURES

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QUANTUM DEVICES WITH 2D SEMICONDUCTORS AND INSULATORS

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COHERENT LIGHT-MATTER INTERACTIONS IN 2D
SEMICONDUCTORS

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LOW-SYMMETRY TWO-DIMENSIONAL STRUCTURES WITH
ANISOTROPIC HIGH CARRIER MOBILITY

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DOUBLE RESONANT RAMAN SCATTERING IN TMDCS

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BCS-BEC CROSSOVER IN A 2D SUPERCONDUCTOR

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DEFECTS AND THEIR INFLUENCE ON THE THERMOELECTRIC
PROPERTIES OF MATERIALS: AN *AB INITIO* STUDY

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MORPHOLOGICALLY DESIGNED NOVEL NANOCARBON MATERIALS
DERIVED FROM HIGHLY STABLE SWCNT INKS

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2D AND TOPOLOGICAL MAGNETIC MATERIALS

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SEMICONDUCTING LAYERED TRANSITION-METAL
DICHALCOGENIDES: INSIGHTS FROM FIRST-PRINCIPLES

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NEW PHOSPHORUS STRUCTURES: FROM TYPE-II RED
PHOSPHORUS TO PHOSPHORENE EDGES

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STACKING AND TWISTING GRAPHENE AND OTHER 2D MATERIALS
FOR QUANTUM NANO-OPTOELECTRONICS

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UNUSUALLY STRONG "HIDDEN" RASHBA EFFECTS IN Si_2Bi_2

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TUNABLE SPIN-ORBIT COUPLING IN A HIGH MOBILITY FEW-LAYER
SEMICONDUCTOR

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DEFECTS AND DEFECT DYNAMICS IN NOVEL 2D MATERIALS

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STRONGLY CORRELATED PHASES OF MATTER IN SEMICONDUCTOR
MOIRÉ SUPERLATTICES

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STRONG LIGHT-MATTER COUPLING IN 2D ATOMIC CRYSTALS

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2D VAN DER WAALS HETEROSTRUCTURES FOR EMERGING DEVICE
APPLICATIONS

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DOPING DEPENDENCE OF TRIONS AND OPTICAL SPECTRA IN MoS_2

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TWO FACES OF A DOUBLE WELL: MULTIFUNCTIONAL DEVICE
BASED ON A Ti_2O MONOLAYER AND MAGNETO-MECHANICAL
SWITCH BASED ON A MXENE NANOTUBE

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CELL POLARITON: A QUANTUM STATE IN THE MYELIN SHEATH OF A
NERVE

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MAGIC OF CARBON ON THE NANOSCALE

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HYBRID 2D AND 3D NANOSTRUCTURED PEROVSKITES: FROM
UNDERSTANDING FUNDAMENTAL PHYSICS TO OPTOELECTRONIC
APPLICATIONS

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STRONG MID-INFRARED PHOTORESPONSE IN TWISTED BILAYER
GRAPHENE

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TUNABLE GRAPHENE SPLIT-RING RESONATORS

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GATE TUNABLE ANISOTROPY IN 2D GATE

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BERRY PHASES IN THE MOIRÉ PATTERNS OF TWISTED TMD
BILAYERS WITH UNIFORM AND NON-UNIFORM STRA

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VIOLET PHOSPHORUS AND PHOSPHORENE

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PAIRING TRANSITION IN INTERACTING ELECTRONIC DOUBLE
LAYERS

Oral Mini-Presentations
(listed by alphabet)

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Mengkun LIU and Vasili
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SCATTERING OF PLASMONS IN CLOSELY PACKED 1D GRAPHENE
STRUCTURES

Tnano 2020

