

US-EU 2D Workshop, October 23-25, 2017, Arlington, Virginia, USA
<http://useu2dworkshop.com>

Final Report submitted to NSF by:
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Executive Summary

The US-EU 2D Workshop was held on October 23-25, 2017 in Arlington, Virginia, USA. Co-organized by the National Science Foundation (NSF) and the European Graphene Flagship Program, this workshop provided a venue for discussion of common challenges and opportunities in this rapidly developing research area. The aim of the workshop was to review recent progress in this rapidly developing research field, to discuss needs and challenges, and to further the strong tradition of collaboration between the U.S. and European Union. This third annual workshop followed prior workshops, in 2016 in Manchester, UK and in 2015 in Arlington, Virginia, USA. The 2017 workshop was sponsored by NSF under Grant EFMA-1748703 and co-organized by US and European researchers co-chaired by Profs. James Hwang (Lehigh University), Alan Seabaugh (University of Notre Dame), Vladimir Falko (University of Manchester), and Frank Koppens (Institute of Photonic Sciences).

The workshop topics ranged widely between graphene and other 2D layered semiconductors such as phosphorene, transition-metal dichalcogenides (TMDs), hexagonal boron nitride, tertiary compounds of carbo-nitrides, and complex oxides. Techniques of scalable synthesis of these materials on multiple substrates and control of layer number and defect density were discussed. The workshop brought together leading scientists from Europe and the United States and government program managers and administrators from the two regions to discuss mechanisms for future collaborations.

As indicated by Prof. Hwang, "There have been several projects formally supported by either the NSF through a supplementary program or the Graphene Flagship through a mobility program. Some of these collaborators will report their results in this workshop. In addition to fundamental physics, material science and novel devices, this workshop emphasizes the integration of graphene and related materials with silicon, which should facilitate their applications."

According to Prof. Falko, "The workshop aims to broaden the scope of 2D material research by studying new materials for applications in optoelectronics and creating new 2D heterostructures. I am aware of two dozen joint papers that Graphene Flagship partners have published in the recent years in collaboration with US colleagues."

The workshop had 87 participants, 66 from the US and 21 from Europe. The participants were primarily from universities and government, including the NSF, the Air Force Office of Scientific Research (AFOSR), the Army Research Lab, the Defense Advanced Research Projects Agency, the Office of Naval Research, the National Institute of Science and Technology, and the European Science Foundation.

The three-day workshop consisted of invited talks interspersed by discussion sessions. The discussion sessions were organized to seek a collective vision on the future of 2D materials, devices, and applications. Discussion session leaders were instructed to engage the attendees in a discussion of the key scientific questions and grand technical challenges in 2D materials. These challenges were at all levels, from first principles modeling, materials synthesis, growth, physics, transport, devices, processes, and integration, to applications.

Discussion Session Findings

Report from Day 1:

Alan Seabaugh, Vladimir Falko, Nikhil Shukla

2D Material Integration. The application of 2D materials will be accelerated by the development of foundry-level deposition techniques like metal-organic chemical vapor deposition (MOCVD), molecular beam epitaxy (MBE), and atomic layer deposition (ALD) techniques for 2D materials on CMOS-compatible substrates. Research is now dominated by exfoliation and layer transfer techniques, which are not readily scalable to 200 to 300 mm substrates. Automated tools are needed. The current state-of-the-art for layer transfer requires a skilled operator. Encapsulation, for example, using transferred BN is also an operator intensive step. Automated encapsulation methods are needed. Industry can develop these methods, but universities should motivate the applications and show the way. Electronic applications, for example the MoS₂ processor development of Thomas Mueller faced challenges related to reproducibility, uniformity, hysteresis, and reliability, which were overcome in the demonstration, but are not solved in general.

Bob Wallace pointed out that the -purity of 2D materials has improved dramatically with the development of MBE and MOCVD approaches. Defects must continue to be studied to improve the purity for electronic and optoelectronic applications. Contacts are also not fully understood e.g. ultrahigh-vacuum deposition of contact metals appears to lower contact resistance vs. common high-vacuum deposition techniques. How are monolayer materials to be cleaned without damaging the surface? We do not yet have a stable doping technique for 2D semiconductors equivalent to ion implantation for precisely setting the layer device doping density.

Continue to Seek Attributes Unique to 2D. Mark Hersham emphasized that there are at least three classes of 2D materials, e.g. MoS₂ (wide bandgap), black phosphorus (narrow bandgap), and borophene (metallic) and given a CVD process these can be integrated with intrinsic new functionality. Grain boundaries in these growths have memristive properties so it is possible to naturally form transistors and memristors in these systems, perhaps for neuromorphic computing applications.

Spin Dynamics and 2D Semiconductor Optical Interactions. Klaus Ensslin discussed current understanding of optical interactions in 2D materials. Fundamental questions remain for utilization of TMDs in optical devices. What is the spectral window for optical gain for laser applications? How should the optical cavity be constructed? What is the role of dark excitons in TMDs? What is their impact on photoemission quantum yield? How robust is the valley degree of freedom in TMDs? Can this be used in valleytronic devices or is it rapidly washed out by intervalley scattering processes? How robust is spin-valley interaction? Can 2D materials play a role in quantum computing? Single photon emitters are not well understood in TMDs and there is a correlation with strain.

Government Investment. According to Dimitris Pavlidis, 2D material and device research is being widely supported by the Division of Electrical, Communications, and Cyber Systems and other divisions of NSF. Multiple programs are underway such as Emerging Frontiers in Research and Innovation Two-Dimensional Atomic-layer Research and Engineering (EFRI-2DARE),

Designing Materials to Revolutionize and Engineering our Future (DMREF), and Materials Innovation Platform (MIP) programs. The EFRI-2DARE program alone is about \$40M and, considering career awards and other NSF investments, the total support of 2D materials and devices is much higher than \$40M. Penn State's 2D Crystal Consortium MIP, another ~\$20M program, accepts user proposals and charges no fee and will synthesize and deliver 2D materials for collaborative experiments. DMREF is another NSF program which supports work in 2D materials under the Materials Genome Initiative to accelerate materials discovery.

Kenneth Goretta pointed out that U.S. Department of Defense supports global investment in basic research. This is an international investment in basic research with few restrictions. Future applications are expected in low-power logic devices, wearables, 2D/3D integration, photodetectors, flexible photonics, chem/bio sensors, and in areas not now envisioned.

Report from Day 2 Breakout Session A:

Eric Pop, Deji Akinwande, Philip Feng

Summary. The application space for 2D materials is broad covering the Internet of things, Industry 4.0, electronics, photonics, and communications. Notable new applications for 2D materials will be in sensing and flexible electronics using roll-to-roll manufacturing. The state of the art in synthesis of 2D materials today uses CVD approaches requiring temperatures $> 800^{\circ}\text{C}$. Graphene can be grown on evaporated Cu up to 12" in diameter (e.g., Aixtron), 4" monolayer MoS_2 is available in polycrystalline form, monolayer hexagonal boron nitride (hBN) is also available. hBN grown on Pt (111) is of sufficient quality for passivation for applications allowing layer transfer. MOCVD growth temperatures are of best quality around 550°C with films at the 4" diameter scale of MoS_2 , MoSe_2 , and WS_2 . MBE with growth temperatures $< 525^{\circ}\text{C}$ has achieved growth on ALD oxides and thermal SiO_2 , e.g. $\text{WSe}_2/\text{HfO}_2/\text{SiO}_2/\text{Si}$, $\text{WSe}_2/\text{SiO}_2/\text{Si}$, $\text{WSe}_2/\text{Al}_2\text{O}_3/\text{SiO}_2/\text{Si}$. ALD TMD films have been grown at $< 350^{\circ}\text{C}$ in nanocrystalline form with mobilities $< 1 \text{ cm}^2/\text{Vs}$.

Synthesis of 2D Materials – Key Questions and Technical Challenges. Methods to grow large area, continuous, single-crystal, monolayer 2D crystals with mobility exceeding $200 \text{ cm}^2/\text{Vs}$ are needed to enable electronic applications; large area growth techniques for graphene and TMDs on hBN could provide high mobility. Conformal growth of TMDs on patterned fins and in vias at temperature $< 450^{\circ}\text{C}$ could open up use in back-end-of-the-line foundry applications. Techniques for layer-by-layer growth of TMD heterostructures are needed. How do grain boundaries impact transport properties? What are the best surfaces for TMD epitaxy? InSe and GaSe are also of interest as they can potentially be grown at low temperatures.

Doping of 2D Materials – Key Questions. The origins of unintentional doping in synthesized 2D materials is not well understood, presumably it is a mixture of impurity doping and electrostatic doping. There are no known techniques for controlling the doping density. How can doping be controlled in 2D materials? A technique like ion implantation or diffusion is needed to precisely control the doping and to form *pn* junctions.

Defects in 2D Materials – Key Questions. Fast, reliable ways to determine and quantify nature and density of defects in 2D crystals are needed. The experimental and theoretical impact of defects on mobility needs to be established. Do transfer processes introduce defects? How do defects evolve over time?

Transfer of 2D Materials – Key Questions. Many groups now have wet and dry transfer methods for graphene, TMDs, and hBN up to 4" in scale. How does transfer conform when the transfers are over steps on the wafer surface? What conformality can be achieved. Is it possible to achieve large-area roll-to-roll stamp transfer from polymer to polymer, and from polymer roll to SiO₂ planar surfaces?

Contacts to 2D Materials – Key Questions. While contacts are being routinely formed, the contacts are metal-semiconductor Schottky contacts. Contact resistances generally need to be lowered by an order of magnitude to < 100 Ωμm. What is the relationship between edge and surface contacts? How does the transfer length depend on layer thickness?

FETs in 2D Materials – Key Questions. Can 2D TMD FETs meet ITRS requirements? Regarding end-of-the-roadmap device scaling and optimization, what is the role of 2D FETs? Can the 2D tunneling FET (TFET) be realized with drive current exceeding 200 μA/μm and $I_{60} > 1 \mu\text{A}/\mu\text{m}$ (highest current at which the subthreshold swing is less than 60 mV/decade). Are vertical interlayer TFETs feasible or is tunneling current too variable, dependent on layer-to-layer misalignment. There are many device concepts in the 2D materials which have yet to be fully investigated: SymFETs, negative-capacitance FETs and TFETs, and ferroelectric gate FETs. Gate stacks and ALD gate dielectrics on TMDs need sustained development. Can equivalent oxide thickness be reduced below 1 nm? 2D FETs for biosensors also needs further development.

Encapsulation of 2D Materials. hBN is now shown to be a successful encapsulant for graphene with record high drift velocity and mobility. hBN is also proving to be a good encapsulant for MoS₂ and other TMDs up to 500°C in air. A deposition technique for encapsulation is needed. ALD dielectrics such as Al₂O₃ have been shown, but these also modify the layer conductivity by doping and can introduce hysteresis.

Emerging Novel Applications of 2D Materials. Many devices are under investigation including topological insulator based devices, thermal transistors, 2D resonant-channel transistors, wearable sensors, memristors, phase-change devices, and nanophotonic devices. Other components benefiting from 2D materials are interconnects, transparent electrodes, and on-chip inductors.

Report from Day 2 Breakout Session B:

Andras Kis, Susan Fullerton, Tania Roy

Summary. This session covered a wide range of topics ranging from fundamental physics to the development of new metrology, to materials growth. The group engaged in a lively discussion of potential new applications, outlined below in "common themes". Even after many years of research on 2D layered materials, the fundamental challenge of wide-area, low defect density, high purity growth remains one of the major discussion topics of this session. While gains have been made, this remains a huge obstacle to progress on applications. Overall, this session highlighted several new and exciting applications that exploit the novel properties that have been uncovered in 2D layered materials.

Common Themes. One major theme of this session was new applications that 2D materials could potentially enable. For example, Andras Kis argued that valleytronics could be exploited to

control Joule heating effects in electronic devices, because even low-power devices will have dissipative currents. Dirk Englund proposed 2D materials to address the need for scalable quantum information processes. Christoph Stampfer proposed a new approach to measuring magnetic fields with 2D materials (e.g., cheap and flexible Hall sensors). Josh Goldberger suggests that 2D materials can make a contribution in the area of magnetics (e.g., room temperature ferromagnets). Gary Steele emphasized the role of graphene in enabling the progress of quantum computers.

A second major theme was the huge gap that still exists between the ability to grow these materials with a semiconductor-quality purity level over wide area. Even though many device applications can be envisioned, the growth and controllable doping strategies simply must catch up. For heterogeneous integration of 2D materials in back-end-of-line CMOS processes, low-temperature growth of 2D materials needs to be established.

Common Challenges. The audience agreed that wide area materials growth is still a huge challenge, and BN was cited as a specific example. Not only do the purity levels need to meet semiconductor requirements, but the substrate itself can introduce doping effects. Albert Davydov emphasized that phase diagrams for TMD compounds and alloys must be reported and used for synthesis and processing. However, comment was made that there is a lack of funding for phase diagram development. A comparison was made to the field of metallurgy, where phase diagrams knowledge and applications are abundant, but there is a gap between metallurgy and electronics. Even beyond the growth, substitutional doping will be required to make electronic devices, and this area is only starting to be explored (e.g., Josh Robinson is exploring Re doping). One particularly attractive feature of 2D layered materials are heterojunctions, but the same growth and purity issues remain. A related challenge is moving the wide-area materials from the growth substrate to another location without organic contamination.

Opportunities for the Future. On the topic of growth, Georg Duesberg points out that a range of 2D materials can be grown below 400°C (e.g., PtSe₂). The question is posed: can there be a one-stop shop for 2D and dielectrics using ALD? Lincoln Lauhon showed some low-temperature growth results on MoS₂ using ALD. Bob Wallace pointed out that low-temperature ALD dielectrics on 2D samples generally suffer from border traps. It is essential to separate the effect of the border traps from interface traps to improve performance and reliability of electronic devices.

Regarding 2D materials processing, one suggestion was that the 2D community should work more closely with the mechanical engineering community to develop technologies for transferring 2D materials without contaminating the surface. For uncovering new properties of 2D materials, the development of new metrology, such as Sam Berweger's scanning microwave microscopy, will be important, in particular because this approach provides insight into the impact of the substrate on the TMD, which was cited above as a specific challenge.

There appears to be a lot of opportunity in the area of 2D materials for scalable quantum information processing, according to Dirk Englund. Imaging techniques have improved to the point that atom-by-atom reconstruction of a material is now possible. In an atomically thin 2D material, the exact location of atoms can be obtained and made use of in density functional theory calculations, which have previously relied heavily on educated guesses. With more

accurate calculations, enabled by precise imaging of atoms, one can make experiments on quantum computation more accurate than was ever possible on conventional 3D systems. According to Gary Steele, graphene junctions have a promising role to play in quantum circuits. Graphene, which is gate-tunable but permits lower current levels than conventional materials used in quantum circuits, can reduce the thermal load and prevent crosstalk, thereby allowing 2D materials to make an impact in this field.

Report from Day 2 Breakout Session C:

Matteo Calandra, William Vandenberghe, Gary Steele

Summary. There is a broad range of physical phenomenon in TMDs which is drawing the attention including fundamental research on spin manipulation, spin transistors, spin-based sensors, ferromagnetic, paramagnetic effects, and light scattering and emission in TMDs and TMD heterostructures. The observation of Moire patterns on TMD multilayers is strong evidence for the realization of atomically clean surfaces. The Moire patterns themselves also reveal the twist on stacked materials. Methods to align transferred layers down to 1° have been shown at the millimeter scale but these need to be scaled up. The angle of stacking between the layers has an impact on physical properties, Raman, and transport and so must be controlled.

Topological insulators – Key questions. What are the effects of electron-electron interactions in 2D topological materials? In contrast to 2D, an advantage of 3D topological insulators is the reduction of electron-electron interactions. What opportunities are there to use 2D materials to make “edges” in the bulk, for example by looking at the atomically sharp transition from single to bilayer exfoliated materials?

Robustness and Reproducibility. Robustness is crucial and is difficult to judge in published work on 2D materials. Many reported results turn out to be not reproducible, even work published in high-impact journals. It is difficult to build on previous work if the device fabrication is not robust or carefully documented, this is a factor slowing progress in the field. A gold standard for this type of research should be reproducibility.

Report from Day 3:

James Hwang, Frank Koppens, Henri Happy

Fundamental Properties. Bart van Wees reported record length spin transport in graphene encapsulated by double-layer hBN instead of Al_2O_3 . For reasons yet unknown, triple-layer hBN did not work. Philip Kim reported the impact on transport by the twisted angle between stacked layers of many 2D materials. Similar effect may appear in MoS_2 and other 2D materials without center symmetry, but it is not yet quantified. It is also possible to separate the effect of size domain and boundaries. Andrea Ferrari reported on 2D heterostructures such as WSe_2 on hBN with clean interface produced by dry transfer without contamination or air bubble.

General Discussion. Large-scale growth and transfer of 2D material remains a key issue. The layers are not likely to be single crystalline so that grain boundaries will be problematic. The issue of transfer vs. direct growth cannot be easily settled and will depend on equipment development and cleanroom compatibility. China and Korea are pushing for equipment development and large-scale integration. Large-area growth and transfer are available today, but defects and contaminants must be reduced to make 2D material compatible with CMOS

integration in cleanroom. How do we go from one to hundreds of devices to millions of devices? Although this may not be exciting to many academic researchers, someone must show the way before industry would be interested to take over.

The relative alignment of transferred 2D layers in heterostructures remains a critical issue. Although automated equipment today can align to within 1° , it needs to be scaled up for large sheets. Both small- and large-angle misalignment may be needed depending on applications. For spintronics, two stacked hBN layers do not work as well as exfoliated bilayer.

Continuing US-EU Collaborations. At least six US-EU collaboration pairs were initiated during this workshop. The nature of collaboration includes material synthesis and characterization, sample exchange, modelling and other theoretical work, student exchange, etc. A common approach for materials standardization was discussed in the wrap up session. This is crucial for gaining industry confidence in the use of graphene and 2D materials and their expected performances. An idea of a web site where information about state-of-the-art performances (characteristics) of materials and devices would be gathered in a bottom-up approach was proposed, but no immediate action was identified. Such an information exchange would require curation/moderation and contributions from the community to be relevant.

Next US-EU 2D Workshop. It will be held in conjunction with the Graphene Week in San Sebastian, Spain September 10-14, 2018 (<http://graphene-flagship.eu/grapheneweek>). This would allow the U.S. researchers and students to get in touch with the large Graphene Flagship community and present the results to the broadest audience. A special session/meeting will be organised probably near the end of Graphene Week to further discuss US-EU collaborations.

Technical Program

US-EU 2D Workshop, Monday, October 23, 2017

	Alan	Seabaugh	U. Notre Dame	Chair
	Vladimir	Falko	U. Manchester	Co-chair
	Nikhil	Shukla	U. Notre Dame	Scribe
0830-0900	Alan	Seabaugh	U. Notre Dame	Welcome and meeting introduction
Session 1	Integration			
0900-0920	James	Hwang	Lehigh U.	Toward 2D-CMOS integration
0920-0940	Frank	Koppens	ICFO, Barcelona	Graphene CMOS camera for visible and infrared light
0940-1000	Thomas	Mueller	TU Wien	2D nanosheet electronics and optoelectronics
Session 2	Challenges in Science and Technology			
1030-1050	Mark	Hersam	Northwestern U.	Interfacial engineering of two-dimensional nanoelectronic heterostructures
1050-1110	Robert	Wallace	U. Texas Dallas	2D materials integration: what have we learned?
1110-1130	Giulio	Cerullo	Milan Polytechnic	Ultra-fast carrier and spin dynamics in 2D semiconductors
1130-1200	All			Discussion - Integration on electronic and optoelectronic platforms
Session 3	Quantum Phenomena			
1330-1350	Klaus	Ensslin	ETH Zurich	2DM quantum devices
1350-1410	Jeremy	Levy	U. Pittsburgh	Correlated nanoelectronics
1410-1430	Alberto	Morpurgo	U. Geneva	Gate induced superconductivity in transition metal dichalcogenides
1430-1500	All			Discussion - What are the major scientific questions that should be addressed?
Session 4	Government Investment Priorities			
1530-1550	Jari	Kinaret	Chalmers U.	Graphene flagship: the present status and future plans
1550-1610	Dimitris	Pavlidis	NSF	2-DARE, MIP, DEMREF and other related investments by NSF
1610-1630	Kenneth	Goretta	AFOSR	Global investment in basic research by the US Department of Defense
1630-1700	Other Government Program Managers			2D-related investments

US-EU 2D Workshop, Monday, October 23, 2017, Poster Session

	Alan	Seabaugh	Notre Dame U.	Chair
	Frank	Koppens	ICFO, Barcelona	Co-chair
1800-2100	Ian	Appelbaum	U. Maryland College Park	Intrinsic two-dimensional states on the pristine surface of tellurium
	Albert	Davydov	NIST	Reversible 2H-1T' phase transformation in MoTe ₂ layers
	William	Douglas	North Carolina State U.	2D TMDC materials foundry and wafer-scale synthesis
	Philip	Feng	Case Western Reserve U.	Highly tunable atomic layer semiconducting 2D nano-electromechanical systems (NEMS)
	Susan	Fullerton	U. Pittsburgh	Monolayer solid state electrolyte for electric double layer gating of 2D field-effect transistors
	Henri	Happy	U. Lille	GFET for high frequency applications: impact of process on high frequency noise
	Tania	Roy	U. Central Florida	Van der Waals heterostructures for energy-efficient electronics
	Alan	Seabaugh	U. Notre Dame	Transistors and steep transistors based on epitaxial 2D-materials, nanoribbons, and nanotubes
	Humberto	Terrones	Rensselaer Polytechnic Inst.	Second harmonic generation of transition metal dichalcogenides alloys and BNC alloys
	Fengnian	Xia	Yale U.	Black phosphorus optoelectronics and electronics
	Kuanchen	Xiong	Lehigh U.	Wafer-scale 2D MOSFET fabrication on CVD MoS ₂ and CMOS substrate
	Xiaodong	Xu	U. Washington	Monolayer magnets
	Wenjuan	Zhu	U. Illinois Urbana-Champaign	Nanoscale electronic and photonic devices based on two-dimensional materials

US-EU 2D Workshop, Tuesday, October 24, 2017, Breakout Session A, Arlington Room

	Eric	Pop	Stanford U.	Chair
	Deji	Akinwande	U. Texas Austin	Co-chair
	Philip	Feng	Case Western U.	Scribe
Session 5A	Vision I			
0830-0850	Kaustav	Banerjee	UC Santa Barbara	2D materials for smart life
0850-0910	Eric	Pop	Stanford U.	Electrical, thermal, and (some) unconventional applications of 2D materials
0910-0930	Deji	Akinwande	U. Texas Austin	Graphene/2D integration: progress, challenges and applications
0930-1000	All			Discussion
Session 6A	Control, Integration, and Oxides			
1030-1050	James	Hone	Columbia U.	Dynamic rotational control of van der Waals heterostructures
1050-1110	Volker	Sorger	George Washington U.	Van der Waals layered materials: building the knowledge-base, synthesis and devices for the new frontier in nanophotonics
1110-1130	Roman	Engel-Herbert	Penn. State U.	Toward integration of 2D materials with functional oxides
1130-1200	All			Discussion
Session 7A	Growth and Metrology			
1330-1350	Christopher	Hinkle	U. Texas Dallas	Back-end-of-line compatible WSe ₂ FETs grown by MBE on ALD oxides
1350-1410	Joan	Redwing	Penn. State U.	Metalorganic chemical vapor deposition of transition metal dichalcogenides
1410-1430	Amalia	Patane	U. Nottingham	From epitaxy to science and technologies of metal chalcogenide van der Waals crystals
1430-1500	All			Discussion
Session 8A	Vision II			
1530-1550	Peide	Ye	Purdue U.	High performance transistor technology enabled by 2D and 1D van der Waals materials
1550-1610	Randall	Feenstra	Carnegie Mellon U.	Limits on the performance of 2D interlayer tunneling field-effect transistors
1610-1630	Spyridon	Pavlidis	Georgia Tech/North Carolina State U.	Towards low-voltage electronic devices using 2D-TMD vertical heterostructures
1630-1700	All			Discussion

US-EU 2D Workshop, Tuesday, October 24, 2017, Breakout Session B, Ballston Room				
	Andras	Kis	EPFL Switzerland	Chair
	Susan	Fullerton	U. Pittsburgh	Co-chair
	Tania	Roy	U. Central Florida	Scribe
Session 5B	Device and Phenomena 1			
0830-0850	Andras	Kis	EPFL Switzerland	Valley/spin devices based on 2D TMDCs
0850-0910	Sam	Berweger	NIST	Microwave near-field imaging of 2D materials and devices
0910-0930	Christoph	Stampfer	RWTH Aachen	Ballistic transport in CVD graphene
0930-1000	All			Discussion
Session 6B	Device and Phenomena 2			
1030-1050	Vladimir	Falko	U. Manchester	Magnetic minibands in moiré superlattices in graphene-hBN heterostructures, persistent to high temperatures
1050-1110	Dirk	Englund	Massachusetts Inst. Technology	2D materials for optoelectronic devices for sensing and communications
1110-1130	Josh	Robinson	Penn. State U.	Creating and exploring atomically-thin materials and heterostructures
1130-1200	All			Discussion
Session 7B	New Materials			
1330-1350	Georg	Duesberg	Trinity C. Dublin	Devices based on PtSe ₂
1350-1410	Albert	Davydov	NIST	Phase diagrams for phase-change and band-gap engineering in TMD materials
1410-1430	Joshua	Goldberger	Ohio State U.	Tailoring electronic and magnetic phenomena in new germanium- and tin-containing 2D materials
1430-1500	All			Discussion
Session 8B	Devices and Heterostructures			
1530-1550	Nikhil	Shukla	U. Notre Dame/ U. Virginia	Controlling filament dynamics in resistive switching devices with 2D interlayers
1550-1610	Lincoln	Lauhon	Northwestern U.	Synthesis and characterization of mixed-dimensional heterostructures
1610-1630	Gary	Steele	Delft U. Technology	Direct observation of the Josephson inductance of a ballistic graphene Josephson junction using a superconducting cavity
1630-1700	All			Discussion

US-EU 2D Workshop, Tuesday, October 24, 2017, Breakout Session C, Clarendon Room				
	Matteo	Calandra	U. Pierre and Marie Curie	Chair
	William	Vandenberghe	U. Texas Dallas	Co-chair
	Gary	Steele	Delft U. Technology	Scribe
Session 5C	Topological Physics and Devices			
0830-0850	William	Vandenberghe	U. Texas Dallas	2D topological insulator electronics
0850-0910	Marco	Polini	Italian Institute of Technology	Recent advances in the fundamental physics of graphene-based van der Waals heterostructures
0910-0930	Peter	Armitage	Johns Hopkins U.	Low frequency electrodynamics of topological materials
0930-1000	All			Discussion
Session 6C	Nanostructures			
1030-1050	Marija	Drndic	U. Pennsylvania	Single nanopores and nanopore arrays in two dimensional materials: science and applications
1050-1110	Radha	Boya	U. Manchester	Atomically smooth angstrom-scale capillaries
1110-1130	Charlie	Johnson	U. Pennsylvania	"Beyond" graphene-enabled bio-nano hybrids for programmable chemical detection
1130-1200	All			Discussion
Session 7C	First Principles Modeling			
1330-1350	Francois	Peeters	U. Antwerp	Turning the electronic properties of phosphorene: straining, stacking, gating and twisting
1350-1410	Kyeongjae	Cho	U. Texas Dallas	DFT and KMC modeling of TMD heterostructures
1410-1430	Alejandro	Strachan	Purdue U.	Ab initio studies of TMDs: new doping avenues and TMD/metal interfaces
1430-1500	All			Discussion
Session 8C	Graphene and More			
1530-1550	Dmitri	Basov	Columbia U.	Polaritons in two-dimensional van der Waals materials
1550-1610	Matteo	Calandra	U. Pierre and Marie Curie	Half-metallic multilayer graphene with rhombohedral stacking
1610-1630	Anupama	Kaul	U. North Texas	Van der Waals solids: enabling advances in printed electronics and photosensing applications
1630-1700	All			Discussion

US-EU 2D Workshop, Wednesday, October 25, 2017

	James	Hwang	Lehigh U.	Chair
	Frank	Koppens	IFCO, Barcelona	Co-chair
	Henri	Happy	U. Lille	Scribe
Session 9	Fundamental Properties			
0830-0850	Bart	van Wees	U. Groningen	Spintronics in van der Waals heterostructures
0850-0910	Philip	Kim	Harvard U.	Commensuration and incommensuration in the van der Waals heterojunctions
0910-0930	Andrea	Ferrari	U. Cambridge	Light scattering and emission from hetero-structures
0930-1000	All			Discussion
Session 10	Conclusion			
1030-1050	Eric	Pop	Stanford U.	Report from breakout session A
	Deji	Akinwande	U. Texas Austin	
	Philip	Feng	Case Western Res.	
1050-1110	Andras	Kis	EPFL Switzerland	Report from breakout session B
	Susan	Fullerton	U. Pittsburgh	
	Tania	Roy	U. Central Florida	
1110-1130	Matteo	Calandra	U. Pierre and Marie Curie	Report from breakout session C
	William	Vandenbergh	U. Texas Dallas	
	Gary	Steele	Delft U. Technology	
1130-1200	All			Discussion

List of Participants



Photo by Dr. Sophia Lloyd

First Name	Last Name	Affiliation
Deji	Akinwande	U. Texas Austin
Ian	Appelbaum	U. Maryland College Park
Peter	Armitage	John Hopkins U.
Chagaan	Baatar	Office of Naval Research
Kaustav	Banerjee	U. California Santa Barbara
Paola	Barbara	Georgetown U.
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Sam	Berweger	National Inst. Standards & Tech.
Radha	Boya	U. Manchester
Matteo	Calandra	U. Pierre and Marie Curie
Eva	Campo	National Science Foundation
Giulio	Cerullo	Milan Polytechnic
Phillip	Chang	DARPA
Kyeongjae	Cho	U. Texas Dallas
Kershed	Cooper	National Science Foundation
Albert	Davydov	National Inst. Standards & Tech.
Miriam	Deutsch	National Science Foundation
William	Douglas	North Carolina State U.
Marija	Drndic	U. Pennsylvania
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Georg	Duesberg	Trinity College Dublin
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Vladimer	Falko	U. Manchester
Randy	Feenstra	Carnegie Mellon U.
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Andrea	Ferrari	U. Cambridge
Lisa	Friedersdorf	National Sci. Tech. Council
Susan	Fullerton	U. Pittsburgh
Joshua	Goldberger	Ohio State U.
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Ana	Helman	European Science Foundation
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Chris	Hinkle	U. Texas Dallas
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Jeremy	Levy	U. Pittsburgh
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Pengke	Li	U. Maryland College Park
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Misoon	Mah	Air Force Office Sci. Res.
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Amalia	Patane	U. Nottingham
Dimitris	Pavlidis	National Science Foundation
Spyridon	Pavlidis	North Carolina State U.
Francois	Peeters	U. Antwerp

Brett	Pokines	Air Force Office Sci. Res.
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Gary	Steel	Delft University of Technology
Alejandro	Strachan	Purdue U.
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Graphene/2D Integration: Progress, Challenges and Applications

ABSTRACT

We will present the progress in graphene growth, transfer, integration and applications. This will include i) wafer-scale growth which has been achieved and commercialized, ii) wafer-scale transfer using 'clean' dry delamination methods for which significant progress has been accomplished and a startup company has formed for commercialization, and iii) wafer-scale metrology using optical and THz methods to quantify important characteristics such as material quality, sheet resistance and mobility mapping. Importantly, mobility mapping suggests graphene grown on Ge offers the most promising for practical integration onto Si platforms. In addition, the smoothness and uniformity of graphene grown on Ge overcomes some of the fundamental obstacles of graphene on Cu substrates.

In addition, the dry transfer integration method is applicable universally to a wide variety of 2D materials including TMDs, Silicene and Xenene, Bismuthene and epitaxial van der Waals atomic sheets. We conclude by showing hybrid platform examples including monolithic integration of graphene onto TSMC Si chips for sensor applications. Other emerging opportunities include 2D wearable sensors for mobile health, fitness and human-machine interfaces.

BIO



Dr. Deji Akinwande received the PhD degree in Electrical Engineering from Stanford University in 2009, where he conducted research on the synthesis, device physics, and circuit applications of carbon nanotubes and graphene. His Master's research in Applied Physics at Case Western Reserve University pioneered the design and development of near-field microwave probe tips for nondestructive imaging and studies of materials.

He is the David & Doris Lybarger Endowed Faculty Fellow and Associate Professor at the University of Texas at Austin. Prof. Akinwande has been honored with the 2017 Bessel-Humboldt Research Award, the U.S. Presidential PECASE award, the inaugural Gordon Moore Inventor Fellow award, the inaugural IEEE Nano Geim and Novoselov Graphene Prize, the IEEE "Early Career Award" in Nanotechnology, the NSF CAREER award, several DoD Young Investigator awards, the 3M Nontenured Faculty Award. His results on silicene have been featured by Nature News, Time Magazine and is the most cited 2015 Nature Nanotechnology paper. His work on flexible 2D electronics was highlighted among the "best of 2012" by the nanotechweb news portal and has been featured on MIT's technology review and other technical media outlets. He is a distinguished lecturer of the IEEE Electron Device Society and an Editor for the IEEE Electron Device Letters and Nature NPJ 2D Materials and Applications. He co-authored a textbook on carbon nanotubes and graphene device physics by Cambridge University Press, 2011, and was recently a finalist for the Regents' Outstanding Teaching Award, the highest teaching award from the University of Texas System.

Intrinsic two-dimensional states on the pristine surface of tellurium [1]

Pengke Li and [Ian Appelbaum](#)

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Atomic chains configured in a helical geometry have fascinating properties, including phases hosting localized bound states in their electronic structure. We show how a zero-dimensional state – bound to the edge of a single one-dimensional helical chain of tellurium atoms [2] – evolves into two-dimensional bands on the c-axis surface of the three-dimensional trigonal bulk. We give an effective Hamiltonian description of its dispersion in k -space by exploiting confinement to a virtual “tellurene” bilayer, and elaborate on the diminished role of spin-orbit coupling. These previously-unidentified intrinsic gap-penetrating surface bands were neglected in the interpretation of seminal experiments, where two-dimensional magnetotransport was otherwise attributed to extrinsic accumulation layers.

[1] Pengke Li and Ian Appelbaum, Intrinsic two-dimensional state on the pristine surface of tellurium, arXiv:1708.07099 (2017).

[2] Pengke Li, Jay D. Sau and Ian Appelbaum, Robust zero-energy bound states in a helical lattice, Phys. Rev. B **96**, 115446 (2017).



Ian Appelbaum is Professor of Physics at the University of Maryland, College Park. He graduated with a B.S. degree in Physics and Mathematics from RPI, and a Ph.D. in Physics from MIT. After a postdoc at Harvard, he built his own lab as faculty in Electrical Engineering at the University of Delaware; he moved his group to UMD in 2009. He is a Fellow of the American Physical Society, "*for advancing the study of spin-polarized electron transport in semiconductors, especially the fundamental processes revealed by coherent and time-resolved spin transport over macroscopic distances in silicon and germanium.*"

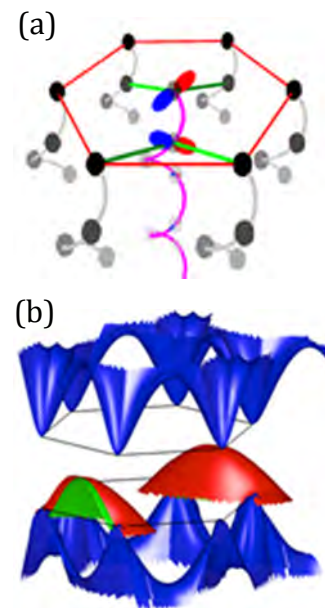


Fig. 1. (a) The c-axis surface state orbitals of the trigonal tellurium lattice made up of 3-fold helical chains. The zero-dimensional bound state, formed from valence p orbitals, is shown in red and blue. (b) Two dimensional tight-binding band structure of the surface states (red and green) penetrating into the band gap between bulk states (blue) .

Low frequency electrodynamics of topological materials

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Topological insulators (TIs) are a recently discovered state of matter characterized by an “inverted” band structure driven by strong spin-orbit coupling. One of their most touted properties is the existence of robust “topologically protected” surface states. The optical response of topological insulators turns out to be one of their most distinguishing and interesting aspects as these materials can be seen not as surface conductors, but as bulk magnetoelectrics. I will review our work on the optical response of topological insulators thin films of Bi₂Se₃ and in particular emphasize our most recent work where we find evidence for Faraday and Kerr rotation angles quantized in units of the fine structure constant. This quantized rotation angle can be seen as evidence for a novel magneto-electric of the TI’s surface states and modified Maxwell’s equations. This quantized rotation is a 3D analog of the quantized resistances seen in quantum Hall systems. The unique optical properties of these materials opens of new areas for photonics applications in the IR regime.



N. Peter Armitage has been on the faculty at Johns Hopkins University since 2006. He received his B.S. in Physics from Rutgers University in 1994 and his Ph.D. from Stanford University in 2002. He is a physicist whose research centers on material systems which exhibit coherent quantum effects at low temperatures, like superconductors and “quantum” magnetism. He is exploiting (and developing) recent technical breakthroughs using very low frequency microwave and THz range radiation to probe these systems at their natural frequency scales. The material systems of interest require new measurement techniques as their relevant frequencies typically fall between the range of usual optical and electronic methods. He has been the

recipient of a DARPA Young Faculty Award, an NSF Career Award, a Sloan Research Fellowship, was a three time Kavli Frontiers Fellow, the William Spicer Award from the Stanford Synchrotron Radiation Laboratory, the William L. McMillan Award from the University of Illinois and 2016 Genzel Prize. He was also the co-chair of the 2014 Gordon Research Conference in Correlated Electron Systems.

2D Materials for Smart Life

Kaustav Banerjee

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Abstract— I will highlight the prospects of 2D materials for innovating energy-efficient transistors, sensors, and interconnects targeted for next-generation electronics needed to support the emerging paradigm of the *Internet of Everything* (Fig. 1). More specifically, I will bring forward applications uniquely enabled by 2D materials and their heterostructures that have been demonstrated in my lab for realizing ultra-energy-efficient electronics. This will include the world's first 2D-material channel band-to-band tunneling transistor that overcomes a fundamental power consumption challenge in all electronic devices since the invention of the first transistor in 1947, as well as a breakthrough interconnect technology based on doped-graphene-nanoribbons, which overcomes the fundamental limitations of conventional metals and provides an attractive pathway toward a low-power and highly reliable interconnect technology for next-generation integrated circuits. I will also bring forward a new class of ultra-sensitive and low-power sensors as well as area-efficient and high-performance passive devices, both enabled by 2D materials, for ubiquitous sensing and connectivity to usher unprecedented improvements in quality of life.

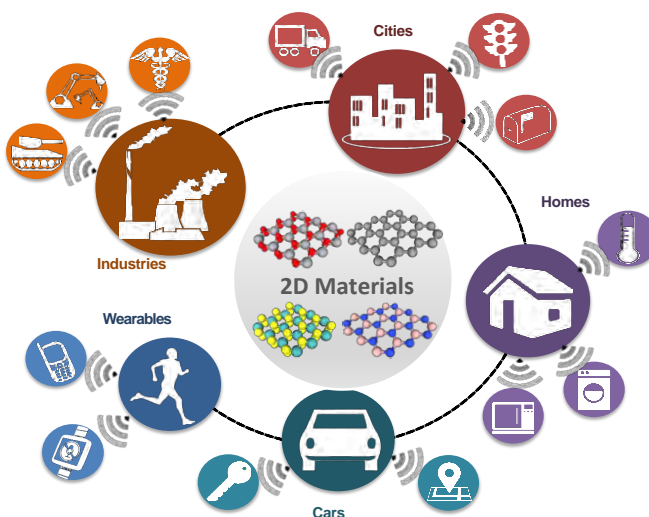


Fig. 1. 2D materials enabled *Internet of Everything* for smart life.



Professor Kaustav Banerjee from UC Santa Barbara is one of the world's leading innovators in the field of nanoelectronics. His current research focuses on the physics, technology, and applications of 2D nanomaterials and their heterostructures for designing next-generation green electronics, photonics, and bioelectronics. Initially trained as a physicist, he graduated from UC Berkeley with a PhD in electrical engineering in 1999.

A Fellow of IEEE, APS, and AAAS, Professor Banerjee has made seminal contributions toward extending the frontiers of energy-efficient electronics. This includes pioneering work on 3D ICs, now being widely commercialized, which has been recognized by IEEE with the *2015 Kiyo Tomiyasu Award*, one of the institute's highest honors. Professor Banerjee's foundational work on contacts/interfaces to 2D materials (*Phys. Rev. X* 2014, *Nature Materials* 2015) and radical innovations with 2D materials are setting the stage for a new generation of ultra-energy-efficient electronics needed to support the emerging paradigm of the "Internet of Everything". This comprised of demonstrating the world's first 2D-material based tunneling transistor that reduces power dissipation by over 90% (*Nature* 2015), as well as a novel energy-efficient interconnect technology based on graphene that also overcomes a fundamental reliability limitation of conventional interconnect materials (*Nano Letters* 2017).

Polaritons in two-dimensional van der Waals materials

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Polaritons are hybrid excitations of light and matter. Van der Waals two-dimensional (2D) materials host a full suite of polaritonic modes originating from light hybridizing with electrons, phonons, excitons and even Cooper pairs [1]. These polaritonic modes reveal the highest degree of confinement among all known materials thus enabling novel avenues for physics research as well as empowering applications based on novel physics principles. For example, phonon polaritons in prototypical 2D material boron nitride [2] are well suited for sub-diffractive focusing and imaging [3], whereas plasmon polaritons in graphene are amenable to both electrostatic and ultra-fast optical manipulation [4]. Polaritonic quasiparticles display or are predicted to display enigmatic quantum effects including condensation and superfluidity, lasing, topological protection, dipole-forbidden absorption [5]. Yet the experimental access to these novel phenomena demands long lifetimes of polaritonic states. Long lifetimes are particularly difficult to achieve for plasmon polaritons. We exploited the nascent technique of cryogenic infrared nano-imaging developed in my group [6] to directly investigate propagating plasmons in high mobility graphene. Our nano-imaging experiments unequivocally show that plasmons in high-mobility structures can propagate ballistically with their travel range restricted only by dimension of macroscopic devices (unpublished). This first observation of ballistic plasmon polaritons in graphene sets the stage for the exploration of non-linear 2D optical phenomena in van der Waals heterostructures as well as for the implementation of chiral edge plasmons that are predicted to reveal highly reduced dissipation rooted in topological protection.

2D materials research at Columbia is supported by ONR, DOE and NSF-EFRI programs.

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Microwave Near-Field Imaging of 2D Materials and Devices

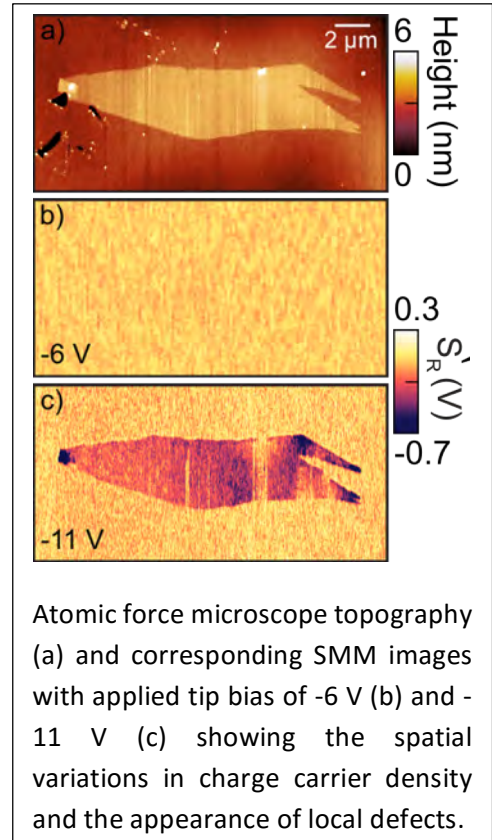
S. Berweger, T.M. Wallis, and P. Kabos

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To further develop and optimize a new generation of devices based on 2D materials and their heterostructures will require techniques capable of directly identifying and studying the effects of structural and electronic inhomogeneities on nanometer length scales. Scanning microwave microscopy (SMM) can measure local variations in sample conductivity at GHz frequencies with nanometer spatial resolution. Here we discuss the applications of SMM to the study of 2D semiconductors, including MoS₂ and WSe₂. By applying a bias to the SMM tip in contact-mode feedback, we modify the sample conductivity and associated contrast to identify and image local electronic inhomogeneities. We perform bias-dependent spectroscopy, which we combine with finite element modeling and simple band structure approximations to identify the local carrier type and density, as well as elucidate the effects of local defects and contaminants. We further demonstrate the application of SMM to the study of 2D semiconductor devices, where we can image spatial variations in charge carrier density during device operation in response to an applied gate voltage.



Dr. Sam Berweger is a postdoctoral researcher at the National Institute of Standards and Technology in Boulder, CO. He graduated with B.S. in Physics from the University of California at Santa Cruz, and received his PhD from the University of Washington. After working as a postdoctoral researcher at the University of Colorado, Boulder, he joined the National Institute of Standards and Technology as a National Research Council (NRC) fellow. His research has focused on the applications and development of scanning probe-based near-field imaging and spectroscopy techniques, encompassing optical methods ranging from tip-enhanced Raman scattering to infrared scattering-type scanning near-field optical microscopy, as well as scanning microwave microscopy. He is particularly interested in low-dimensional and correlated electron materials.

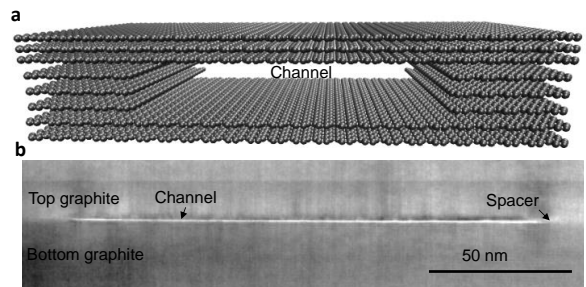
Atomically Smooth Angstrom-Scale capillaries

B. Radha, A. Esfandiari, F. C. Wang, A. P. Rooney, K. Gopinadhan, A. Keerthi, A. Mishchenko, A. Janardanan, P. Blake, L. Fumagalli, M. L. Hidalgo, S. Garaj, S. J. Haigh, I. V. Grigorieva, H. A. Wu & A. K. Geim

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It has been an ultimate but seemingly distant goal of nanofluidics to controllably fabricate capillaries with dimensions approaching the size of small ions and water molecules. Nanometre-scale pores and capillaries have long been studied because of their importance in many natural phenomena and their use in numerous applications. A more recent development is the ability to fabricate artificial capillaries with nanometre dimensions, which has enabled new research on molecular transport and led to the emergence of nanofluidics. But surface roughness in particular makes it challenging to produce capillaries with precisely controlled dimensions at this spatial scale. We have developed a method for fabrication of narrow and smooth capillaries through van der Waals assembly, with atomically flat sheets at the top and bottom separated by spacers made of two-dimensional crystals with a precisely controlled number of layers. Water transport through the channels, ranging in height from one to several dozen atomic planes, is characterized by unexpectedly fast flow (up to 1 metre per second) that we attribute to high capillary pressures (about 1,000 bar) and large slip lengths. For channels that accommodate only a few layers of water, the flow exhibits a marked enhancement that we associate with an increased structural order in nanoconfined water. Our work opens up an avenue to making capillaries and cavities with sizes tunable to ångström precision, and with permeation properties further controlled through a wide choice of atomically flat materials available for channel walls. Our results lay the basis for exploration of such Å-size slits in nanofluidics, molecular separation and other nanotechnologies.

Fig. 1. **Graphene capillary device.** **a**, General schematic of devices. The arrow indicates the molecular flow direction. **b**, Scanning electron microscopy (SEM) image of a trilayer device ($h \approx 1.0$ nm; top view). One can discern that the spacers (dotted lines) run under the top graphite layer all the way to the hole etched in the bottom graphite. Its edge is indicated by the dashed line.



b, Cross-sectional bright field image of a bilayer capillary ($h \approx 7$ Å) in a scanning transmission electron microscope.



Radha Boya is a Leverhulme early career fellow in condensed matter physics group, at the University of Manchester (UoM) where she is exploring the fundamentals and applications of atomic scale nanocapillaries. She has been funded through a series of highly competitive and prestigious fellowships, held at Northwestern University (Indo-US pre- and postdoctoral fellowship), UoM (Marie Curie international and Leverhulme early career fellowship). She has published 37 research papers including those in *Nature* and *Science* journals. Recently, she was named as UNESCO L'Oréal-women in science fellow and was recognized as an inventor in MIT Technology Review's "Innovators under 35" List.

Half-metallic multilayer graphene with rhombohedral stacking

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Attempts to induce a clean and stabilized gap in the excitation spectrum of graphene, or a robust magnetism preserving a high carrier mobility have not been successful yet. An alternative procedure to achieve an optical gap and a magnetic state in graphene is to explore correlated states in flat electronic bands hosted by multilayer graphene with rhombohedral stacking [1]. The low kinetic energy of such carriers could lead to gap opening even at weak Coulomb repulsion by stabilizing a magnetic or superconducting state. Here, we directly image the band structure of large graphitic flake containing approximately 14 consecutive ABC layers. We reveal the flat electronic bands and identify a gapped magnetic state by comparing angle-resolved photoemission spectroscopy with first-principle calculations [2]. Finally, by simulating the effect of the electric field on the sample in a field effect configuration we show that a perfect half-metallic behavior can be induced in the ABC multilayers [3].

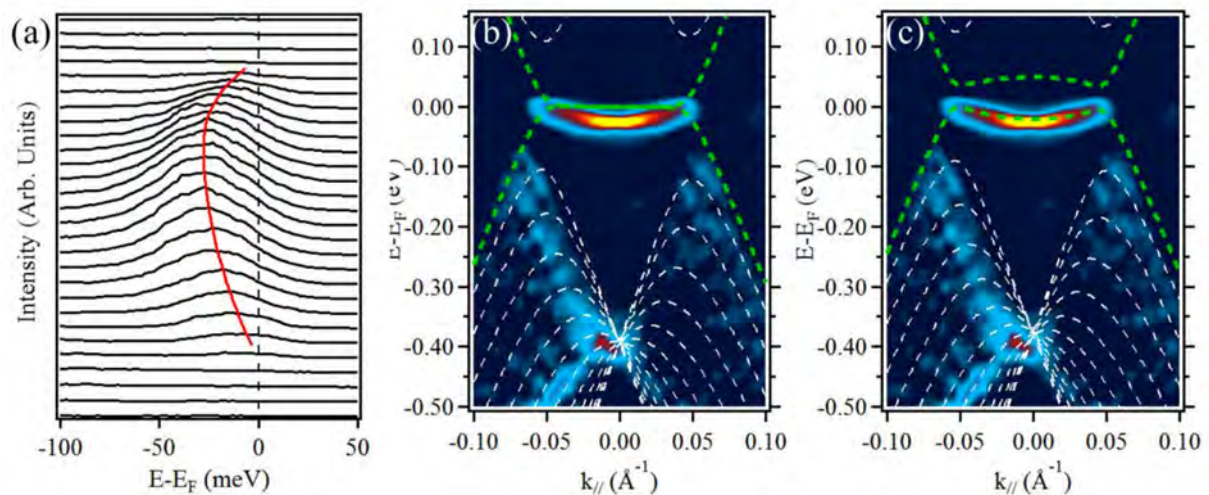


Fig. 1 ARPES measured electronic structure (a,b,c) compared with non-magnetic (b) and magnetic (c) first principles calculations including exact exchange.



Matteo Calandra is research director at CNRS and Université P. et M. Curie. He graduated with a B.S. degree at the University of Parma (Italy) and then obtained his PhD in theoretical condensed matter physics at the International School for Advanced Studies (SISSA/ISAS) in Trieste. He has been postdoc in Stuttgart at Max Planck Institut für festkörperforschung and he has been visitor in Gerogetown University, Naval Research Lab, RIKEN, and Università di Roma La Sapienza. He has published 92 papers cited more than 9000 times with impact factor $h > 33$. His research activity involves the developments of new theoretical methods in the field of first principles electronic structure calculations as well as the study of electronic structure, vibrational and transport properties of solids and 2D materials.

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Ultrafast carrier and spin dynamics in 2D semiconductors

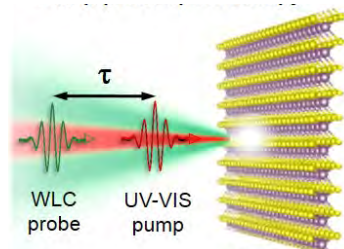
S. Dal Conte, Z. Wang, E.A.A. Pogna, P. Altmann, C. Trovatiello and G. Cerullo

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We discuss the ultrafast optical response of transition metal dichalcogenides (TMDs), focusing on two aspects: time-resolved measurements of exciton dynamics and spin/valley relaxation processes. We first study exciton dynamics in single-layer MoS₂ by femtosecond transient absorption spectroscopy over a broad photon energy range. The non-equilibrium optical response is characterized by prominent features, each consisting of a bleaching at the energy of the excitonic transition and a red-shifted photoinduced absorption, independent of the excitation energy. The experimental data are compared with first-principle simulations that combine non-equilibrium Green's functions with density-functional theory methods. The comparison shows that the mere Pauli blocking effect of the photoexcited transition cannot account for the experimental results. Instead, a bandgap renormalization process, i.e. a transient reduction of the quasi-particle optical gap and the exciton binding energy caused by the presence of photo-excited carriers, can quantitatively reproduce the MoS₂ non-equilibrium optical response. We then use two-colour helicity-resolved pump-probe spectroscopy in order to disentangle the intervalley and intravalley spin-flip processes of electrons in the conduction band of single-layer WS₂. Spin-polarized carriers are injected by a circularly polarized pump pulse resonant with the A exciton, while the co-circularly polarized probe pulse is tuned around the B excitonic peak. In this configuration, the scattering of the electrons from the upper to the lower conduction band level (where they cannot radiatively recombine) is detected by measuring the build-up dynamics of the bleaching signal around the B exciton caused by Pauli blocking. We also show that spin-conserving intervalley scattering dynamics occur on a faster time-scale than the intraband spin-flip process.



co-circularly polarized probe pulse is tuned around the B excitonic peak. In this configuration, the scattering of the electrons from the upper to the lower conduction band level (where they cannot radiatively recombine) is detected by measuring the build-up dynamics of the bleaching signal around the B exciton caused by Pauli blocking. We also show that spin-conserving intervalley scattering dynamics occur on a faster time-scale than the intraband spin-flip process.

Fig. 1. broadband ultrafast optical spectroscopy of single-layer TMDs.



Giulio Cerullo is a Full professor with the Physics Department, Politecnico di Milano, where he leads the Ultrafast Optical Spectroscopy laboratory. Prof. Cerullo's research activity covers a broad area known as "Ultrafast Optical Science", and concerns on the one hand pushing our capabilities to generate and manipulate ultrashort light pulses, and on the other hand using such pulses to capture the dynamics of ultrafast events in molecular and solid-state systems. He has published more than 350 scientific papers on renowned international journals, which received 15000 citations (H-index: 64). Since 2014 he is a Fellow of the Optical Society of

America. He is the recipient of an ERC Advanced Grant (2012-2017) on two-dimensional electronic spectroscopy of biomolecules. He is responsible for the ultrafast optical spectroscopy activities in the Optoelectronic workpackage of the Graphene Flagship project. He is General Chair of the conferences CLEO/Europe 2017 and Ultrafast Phenomena 2018.

DFT and KMC Modeling of 2D TMD Heterostructures

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Abstract

Over the last three decades, nanoscale materials have been extensively investigated for both academic research and practical industrial applications. Nanomaterials are broadly classified by the number of nanoscale dimensions of the material systems (in practice, indicated by the number of macroscopic dimensions): 0D (fullerenes and nanoparticles) [1], 1D (nanotubes and nanowires) [2], and 2D (graphene, h-BN, TMDs) [3,4] nanomaterials. In this talk, I will discuss about the modeling research on 2D materials, with emphasis on transition metal dichalcogenides (TMDs). 2D compound semiconductors (TMDs; MX_2 with M = transition metal, X = chalcogen) are the recent focus of diverse research activities as a promising 2D device materials. TMDs are covalently bonded 2D layers stacked together with weakly interacting van der Waals gaps, and there have been diverse TMD samples prepared by exfoliation, CVD and MBE growth for material study and device applications. In spite of such increasing research activities, their material properties and how to control them within device structures are not fully understood yet, and topics of ongoing research. To explore possible materials properties and to facilitate the experimental device material development efforts, we have applied predictive *first principles modeling* method to examine TMD materials properties. We have performed predictive density functional theory (DFT) studies of TMD material properties including band alignments in heterostructures, TMD-metal contacts, TMD-oxide interface, and TMD defect and dopant properties.[5,6,7,8,9,10] Furthermore, to guide the experiment efforts to grow high quality TMD samples, we have investigate the kinetics of precursor reactions and the nucleation and growth of TMD samples using DFT and kinetic Monte Carlo simulations.[11,12] In this talk, we will discuss the calculated the atomic and electronic structure information of TMDs and their heterostructures, controlled growth of TMD samples, and their implications for nanoscale device applications in the context of close collaboration with experimental research groups.

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Phase Diagrams for Phase-Change and Band-Gap Engineering in TMD Materials

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Phase diagrams describe thermodynamic equilibrium between various phases as a function of temperature (T), pressure (P), and chemical composition (x). In the case of **TM-X** (where **TM** is a transition metal and **X** is a chalcogen) binary and multi-component systems, phase diagrams define the T - P - x stability range for TMD compounds (e.g., for MoTe_2) and related alloys such as $\text{Mo}_{(1-x)}\text{W}_x\text{Te}_2$. Knowledge of the phase stability field helps to design experiments

to switch from one phase to another, such as to reversibly transform between semiconducting 2H to metallic 1T' phases in Mo-Te and Mo-W-Te systems (see Fig. 1), and to control a band-gap in TMD alloys by tuning their composition. Additionally, phase diagrams define non-stoichiometry limits in TMD compounds, e.g., a concentration of tellurium vacancies V_{Te} in MoTe_{2-x} , which in turn affects conductivity type and charge carrier concentration in semiconducting 2H phase.

This talk demonstrates few examples of both experimental and computational phase diagrams for TM-X systems to illustrate how this knowledge enables engineering of structural and electronic properties in TMD compounds and alloys.

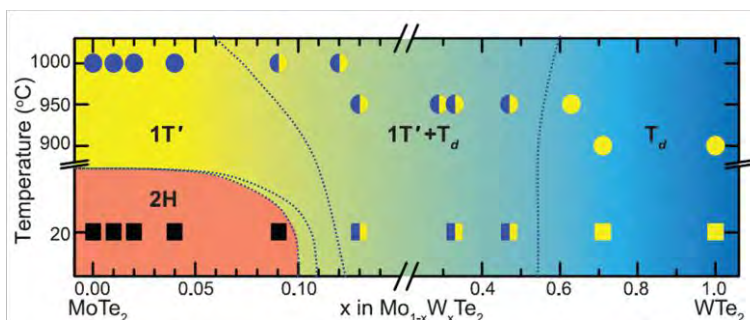


Fig. 1 Experimental MoTe_2 - WTe_2 phase diagram [Oliver et al., 2D Mater. (2017) 4 045008]



Albert Davydov is a Staff Scientist at the National Institute for Standards and Technology (NIST). He received his Ph.D. in Chemistry from Moscow State University (Russia) in 1989. He joined NIST fulltime in 2005 and is now active in the area of semiconducting thin films, nanowires and 2D materials. Dr. Davydov has more than 30 years of experience and over 100 publications with H-factor=32, related to growth of bulk crystals, deposition of thin films, and the fabrication, characterization, and processing of a wide range of nanostructured electronic materials. His expertise also includes thermodynamic modeling and experimental study of phase diagrams for metal and semiconductor material systems.

Davydov is a Leader of Functional Nanostructured Materials Group and a Project Leader on “Low-dimensional semiconductors for sensors, optoelectronics and energy applications” at Materials Science & Engineering Division at Material Metrology Laboratory at NIST. He also serves as a Head of the Semiconductor Task Group for the International Centre for Diffraction Data, co-Chair of the Reference Materials Task Group at ASTM Subcommittee on Compound Semiconductors, and co-Chair of SPIE Optics & Photonics Conference on Low-dimensional Materials and Devices.

POSTER: Reversible 2H-1T' Phase Transformation in MoTe₂ Layers

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Molybdenum ditelluride (MoTe₂), which can exist in a semiconducting prismatic hexagonal (2H) or a metallic distorted octahedral (1T') phases, is one of the very few materials that exhibit reversible metal-semiconductor transition. Temperature-driven 2H → 1T' phase transition in bulk MoTe₂ occurs at high temperatures (above ~900 °C) and it is usually accompanied by Te loss. The latter can exacerbate the control over reversibility of the phase transition.

Here, we study effects of high-temperature annealing on the 2H ↔ 1T' phase transition in MoTe₂ single crystals. First, MoTe₂ were grown in sealed evacuated quartz ampoules from polycrystalline MoTe₂ powder in an iodine-assisted chemical vapor transport process at 1000 °C. The 2H and 1T' phases were stabilized by controlling the cooling rate after the growth. In particular, slow cooling at 10 °C/h rate yielded the 2H phase whereas the 1T' phase was stabilized by ice-water quenching. Next, the reversible phase transformation between 2H and 1T' was achieved by annealing MoTe₂ single crystals in vacuum-sealed ampoules at 1000 °C with or without additional polycrystalline MoTe₂ powder followed by fast or slow cooling. Similarly to the CVT growth, slow cooling and quenching consistently produced 2H and 1T' phases, respectively, regardless of the initial MoTe₂ crystal structure.

This poster discusses structural and optical properties of the as-grown and phase-converted MoTe₂ single crystals using TEM, SEM/EDS, XRD, XPS and Raman. Electrical characteristics of two-terminal devices made from metallic 1T' and bottom-gated FETs made from 2H exfoliated crystals are presented.



Albert Davydov is a Staff Scientist at the National Institute for Standards and Technology (NIST). He received his Ph.D. in Chemistry from Moscow State University (Russia) in 1989. He joined NIST fulltime in 2005 and is now active in the area of semiconductor thin films, nanowires and 2D materials. Dr. Davydov has more than 30 years of experience and over 100 publications with H-factor=32, related to growth of bulk crystals, deposition of thin films, and the fabrication, characterization, and processing of a wide range of nanostructured electronic materials. His expertise also includes thermodynamic modeling and experimental study of phase diagrams for metal and semiconductor material

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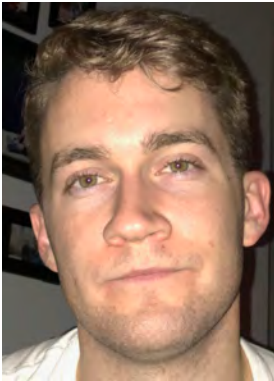
2D TMDC Materials Foundry and Wafer-Scale Synthesis

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ABSTRACT

Atomix Inc (d.b.a 2Dlayer) is dedicated to providing 2D TMDC materials with the highest quality to academia and industry. Our in-house technicians have developed unique synthetic capabilities for single crystalline 2D TMDC flakes, wafer-scale 2D TMDC material films and 2D TMDC material heterostructures. We have already supplied 2D TMDC materials to researchers in academia institutes and international companies around the world. Additionally, 2DLayer has worked closely with academic researchers and industry to develop solutions to accommodate specific research needs. We are committed to helping move the field of 2D materials forward by providing the best solutions of material preparation.

BIO



William H. Douglas graduated from NC State's College of Textiles in May 2016 with a focus in entrepreneurship. Starting 2 businesses in school, William left his work to join 2DLayer in January 2017, and was promoted to Director of Operations in July.

Now studying independently at NC State, he focuses on 2D TMDC synthesis, characterization, and application.

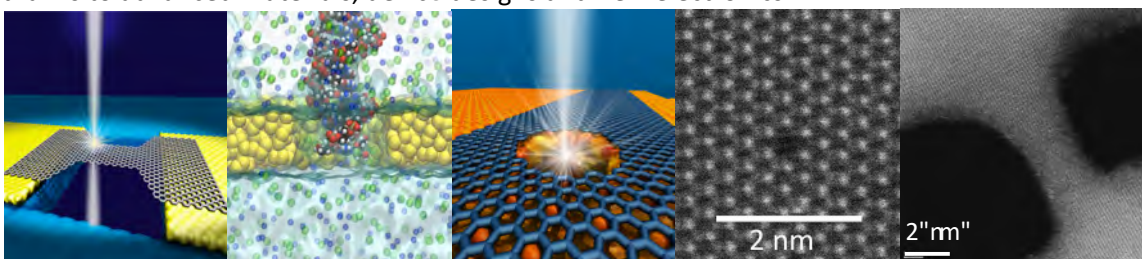
William is particularly intrigued by the vast array of potential applications for TMDCs, and is working to bring 2DLayer closer to wafer-scale commercialization, while providing quality 2D materials to the academic realm.

Single nanopores and nanopore arrays in two dimensional materials: science and applications

Marija Drndic

University of Pennsylvania

I will describe experiments that push the limits of nanoelectronics device size to atomic scale in thin materials and expand their function and precision. Examples include nanoribbons and field-effect-transistors with nanopores from novel two-dimensional materials down to sub-nm widths and the ultrafast, all-electronic detection and analysis of biomolecules, as well as nanopore arrays for filtering applications. As molecules are driven through nanopores in solution, they block the ion current flow resulting in current reductions from which molecule's physical and chemical properties are inferred. DNA, proteins and other biomolecules can be analyzed. Nanopore arrays can be envisioned for efficient water desalination. The temporal, spatial resolution and sensitivity in nanopore experiments have been improved over the last few years thanks to advanced materials, device designs and new electronics.



From left to right: Illustrations of nanoribbon sculpting with the electron beam; passage of a DNA molecule through a nanopore; illustration of nanopore drilling with an electron beam inside of the TEM; one-atom-large nanopore in a MoS₂ sheet; armchair phosphorene nanoribbon sculpted in the AC-TEM. References: G. Danda, *ACS Nano* 11 (2), 1937, 2017; Rodriguez-Manzo *et al.*, *ACS Nano* 10 (4), 4004, 2016 & *ACS Nano* 9 (6), 6555, 2015; Qi *et al.*, *ACS Nano* 9(4), 3510, 2015; Balan *et al.*, *Nano Letters* 14 (12), 7215, 2015; Drndic, *Nature Nanotechnology* 9, 743, 2014.



Marija Drndic is the Fay R. and Eugene L. Langberg Professor in the Department of Physics and Astronomy at the University of Pennsylvania and the faculty member of the MRSEC Center at Penn. She received her Masters from Cambridge University, PhD from Harvard University and was a Pappalardo Fellow at Massachusetts Institute of Technology, before joining Penn in 2003. Her work on nanocrystal electronics and nanofabrication has been recognized by the Presidential Young Investigator Award, the Alfred Sloan Fellowship, the DARPA Young Faculty Award, the ONR Young Investigator, and the NSF Career Award. In 2013 she was named the APS Fellow “for development of novel nanofabrication methods for graphene nanoelectronics and fast biomolecular analysis in solution”. She also received several teaching awards, including the Edmund J. and Louise W. Kahn Award for Distinguished Teaching. The research in the Drndic lab focuses on the exploration of mesoscopic and nanoscale structures in the areas of experimental condensed matter physics, nanoscience and nanotechnology. The group is known for their studies of fundamental physical properties of low-dimensional and small-scale structures and the development of their device applications.

Devices based on PtSe₂

Georg S. Duesberg^{1,2}

Chanyoung Yim, Georg S. Duesberg

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Cormac Ó Coileáin, Katie O'Neil, John, McManus, Conor Cullen, Kangho Lee, Niall McEvoy, G.S. Duesberg

School of Chemistry, Centre for Adaptive Nanostructures and Nanodevices (CRANN) & Advanced Materials BioEngineering Research Centre (AMBER), Trinity College Dublin, Ireland

Two-dimensional transition metal dichalcogenides (TMDs) are intensively investigated owing to their unique properties, which make them of great interest for both fundamental studies and emerging applications. So mainly group six (Mo/W) TMDs have been investigated, while very little is known about group 10 TMDs. In particular, PtSe₂ has drawn attention due to its unique electronic property whereby theoretical studies proposed a transition from semimetal to semiconductor as the layer number decreases. In the presentation we outline the synthesis of PtSe₂ by thermally assisted conversion (TAC) of Pt films. The synthesis is possible below 450°C allowing BEOL integration with silicon technology. The composition and morphology is shown by several characterization techniques including Raman spectroscopy, X-ray photoelectron spectroscopy and transmission electron microscopy. As large scale film and pre-patterned structures can be grown the methodology allows to fabricate electronic devices. Examples for high performance sensors, photodetectors and a photovoltaic cell with PtSe₂ will be given. [1]

[1] High-Performance Hybrid Electronic Devices from Layered PtSe₂ Films Grown at Low Temperature", Chanyoung Yim, Kangho Lee, Niall McEvoy, Maria O'Brien, Sarah Riazimehr, Nina C. Berner, Conor P. Cullen, Jani Kotakoski, Jannik C. Meyer, Max C. Lemme, and Georg S. Duesberg, ACS Nano, 10(10), 9550-9558, (2016)

G.S. Duesberg Universität der Bundeswehr, Neubiberg



Prof. Duesberg's research focuses on making novel devices to exploit the unique properties of low-dimensional structures. These include carbon nanotubes, graphene and other 2D materials. For the integration with silicon technology, functional materials are synthesized and integrated with state-of-the-art micro-processing techniques. The resulting hybrid devices aim towards the use in ICT, sensing and photonics as well as energy conversion and storage.

Prof. Georg S. Duesberg graduated in Physical Chemistry from the University of Kassel, Germany in 1996. He was researcher at the Max-Planck-Institute for Solid State Research, Stuttgart and Trinity College Dublin from 1997 – 2001 after which he received his PhD from the University of Tübingen in 2001. From 2001 – 2005 he worked at the Infineon AG, in the Corporate Research Department in Munich. From 2005 – 2007 Prof. Duesberg was in the Thin Films Department at Qimonda AG, Dresden. In 2007 Prof. Duesberg became of member the School of Chemistry and Principal Investigator in Centre for Adaptive Nanostructure and Nanodevice (CRANN) at Trinity College Dublin. In 2017 Prof. Duesberg took on the Chair for Sensortechnologies at the Universität der Bundeswehr in Neubiberg. He has co-authored more than 200 publications with more than 13000 citations (Reuters, H-index 51) and has filed more then 25 patents.

Toward integration of 2D materials with functional oxides

M. Hilse, J.R. Robinson, J.M. Redwing, and R. Engel-Herbert
The Pennsylvania State University, University Park, PA 16802

The highly anisotropic nature of bond geometry in transition metal chalcogenide compounds not only allows to stabilize atomic layer thin sheets of these materials. The synthesis of artificially layered materials with different stacking sequence provides access to a plethora of materials configurations in a largely unexplored material design space, which becomes even larger if integrated with functional oxides. Exotic properties emerging from proximity coupling across dissimilar heterointerfaces are expected, however these novel states of matter can only be understood and harnessed if a controlled synthesis of these hybrid structures is possible. Within the scope of the Materials Innovation Platform (MIP) Center at Penn State the prediction, synthesis and characterization of these material system can be realized. We present capabilities and opportunities available to the user community of this NSF-funded center and discuss their realization by presenting different examples.

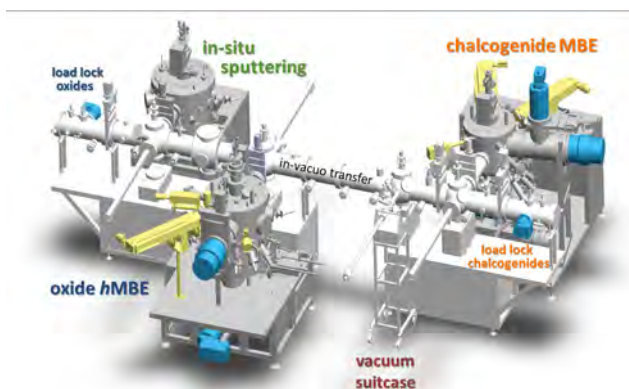


Figure 1. Synthesis capability available through the 2DCC-MIP center at Penn State to integrate 2D atomic layer materials and functional oxides.

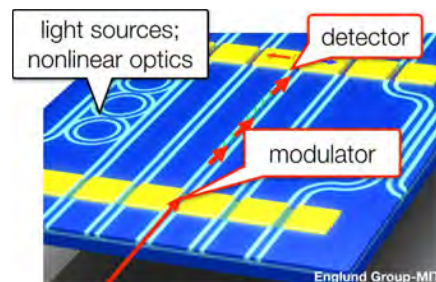


Dr. Roman Engel-Herbert is Associate Professor in the Departments of Materials Science and Engineering and Chemistry at the Pennsylvania State University. He received the Dipl.-Phys. (M.Sc.) degree in Physics from the Friedrich-Schiller-University Jena, Germany, in 2002 and the Dr. rer. nat. (Ph.D.) degree in Experimental Physics from Humboldt University Berlin, Germany in 2006. After a short stay as a visiting scientist in the ECE Department at the University of Waterloo, Canada, and a postdoctoral position in the Materials Department at the University of California Santa Barbara from 2007 to 2010, he joined the Materials Science and Engineering Department at the Pennsylvania State University. He is recipient of the Tech Connect Innovation Award in 2016, NSF CAREER award (2014), the Rustum and Della Roy Innovation in Materials Award (2014), a Feodor Lynen fellowship of the Humboldt Foundation (2008-09), and the Carl Ramsauer Award of the Physical Society of Berlin (2006), and has published over 70 referred papers. He has researched the development of high-k dielectrics on compound semiconductors for beyond Si CMOS technology and is currently working on oxide materials with strong electron correlation effects to utilize them in electronic and photonic devices. His current research is focused on the synthesis of chalcogenide and oxide thin films targeted at developing novel artificial materials.

2D Materials for Optoelectronic Devices for Sensing and Communications

Dirk Englund, EECS, MIT

There has been great experimental progress towards a range of emerging quantum technologies, but new device concepts are needed to achieve the required quantum control of light and matter. Recent work shows that different types of 2D materials can be assembled into entirely new types of 2D heterostructures, enabling optoelectronic properties that were impossible using bulk semiconductors. These atomically engineerable heterostructures hold particular promise for quantum technologies. Here, we review our recent work in two application areas. The first part of the talk focuses on chip-integrated graphene photodetectors. Depending on the different photodetection processes available in graphene, waveguide-integrated detectors can attain high response speed and responsivity [1], and they also promise single-photon resolution across a broad optical spectrum[2]. The second part of the talk focuses on light sources, including spectrally tunable thermal[3] and spectrally tunable single-photon sources[4,5].



Dirk Englund received his BS in Physics from Caltech in 2002. Following a Fulbright year at TU Eindhoven, he earned an MS in electrical engineering and a PhD in Applied Physics in 2008, both from Stanford University. He was a postdoctoral fellow at Harvard University until 2010, when he started his group as Assistant Professor of Electrical Engineering and of Applied Physics at Columbia University. In 2013, he joined the faculty of MIT's Department of Electrical Engineering and Computer Science. Dirk's research focuses on quantum technologies based on semiconductor and optical systems. Recent recognitions include the 2011

Presidential Early Career Award for Scientists and Engineers, the 2011 Sloan Research Fellowship in Physics, the 2012 DARPA Young Faculty Award, the 2012 IBM Faculty Award, an 2016 R&D100 Award, the OSA's 2017 Adolph Lomb Medal, and the 2017 ACS Photonics Young Investigator Award.

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- [3] R.-J. Shiue, Y. Gao, C. Peng, C. Tan, D. K. Efetov, Y. D. Kim, J. Hone, and D. R. Englund, in *Conference on Lasers and Electro-Optics* (OSA, Washington, D.C., n.d.), p. STu4F.5.
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- [5] Yaqing Bie, Gabriele Grosso, Mikkel Heuck, Marco Furchi, Yuan Cao, Jiabao Zheng, Darius Bunandar, Efren Navarro-Moratalla, Lin Zhou, Dmitri Efetov, Takashi Taniguchi, Kenji Watanabe, Jing Kong, Dirk Englund, and Pablo Jerillo-Herrero, to appear in *Nature Nanotechnology* (2017)

2D Quantum Devices

H. Overweg, M. Eich, R. Pisoni, Y. Lee, P. Rickhaus, A. Ijaz, T. Ihn and K. Ensslin
ETH Zurich, Switzerland

2D crystals are ideal systems for the realization of strongly confined quantum structures. Many experiments over the last years have focused on etched graphene quantum devices because of the missing band gap. Most devices were dominated by localized states along the graphene edges which are difficult to control on the atomic scale.

In this talk I will present two solutions to this problem. In bilayer graphene a bandgap arises for vertical electric field. We demonstrate that a split-gate arrangement can be used to define a narrow 1D ballistic channel displaying quantized conductance. Using 1D pnp and npn junctions we realize quantum dots with single electron and single hole occupancy. Excited spectroscopy and magnetic field dependence of the ground state energies allows to extract level degeneracy, Zeeman splitting and valley splitting. Another approach is based on MoS₂ encapsulated between layers of BN to obtain best electronic quality. At low magnetic fields we observe a degeneracy of 6, which is explained by the 6-fold valley (Q valley) degeneracy in the conduction band of MoS₂. In a quantum point contact again conductance pinch-off and plateau-like features are observed.

2D materials have improved to an extent, that novel electronic quantum devices can be realized with great promise.



Klaus Ensslin is professor of physics at ETH Zurich since 1995. Since 2011 he is the director of the Swiss National Competence Center on “Quantum Science and Technology”.

The research of Klaus Ensslin focuses on quantum devices in semiconductor structures as well as 2D materials. The lab is specialized on ultra-sensitive electrical measurements that allow to do transport spectroscopy of electronic quantum systems down to carrier temperatures of 10 mK.

Klaus Ensslin is a fellow of the American Physical Society.

Magnetic minibands in moiré superlattices in graphene-hBN heterostructures, persistent to high temperatures

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When graphene lattice is aligned with the hBN lattice, a long-wavelength periodic moiré pattern forms due to a weak incommensurability of the two lattice structures, leading to a long-range superlattice affecting properties of electrons in graphene. At weak fields, electron states form minibands with peculiar properties [1,2]. At high magnetic fields, electron spectrum transforms into a fractal sequence of Brown-Zak magnetic minibands [3], which emerge from Landau levels at low magnetic field and develop [4] into ‘Hofstadter butterfly’ [5] type spectra. For graphene-hBN heterostructures, the experimentally available magnetic fields are sufficient to provide flux BS through the moiré superlattice cell comparable to the magnetic flux quantum φ_0 and to observe the manifestation of magnetic minibands in magneto-transport and magneto-capacitance measurements [2]. These minibands display a hierarchy of their band properties (in particular, characteristic group velocity in the band) which is reflected in $1/B$ magneto-oscillations persistent to the high temperatures [6].

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Professor Vladimir Falko (in publications, Fal'ko) is Director of the National Graphene Institute and Head of Theory Division in the School of Physics and Astronomy at the University of Manchester. He is also the Editor in Chief of the IoP Journal ‘2D Materials’ and head of Division 1 in the European Graphene Flagship.



Limits on the Performance of 2D Interlayer Tunneling Field-Effect Transistors

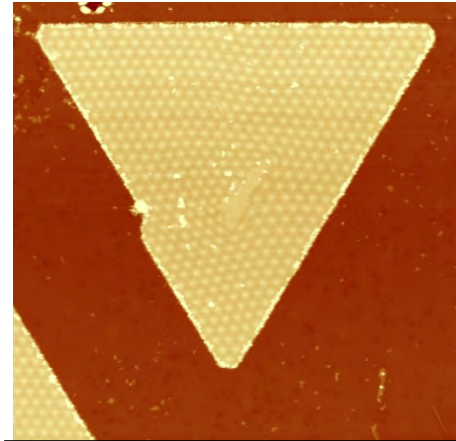
Randall Feenstra

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Interlayer tunneling field-effect transistors (TFETs) are devices in which the tunnel current flows vertically between two layers of two-dimensional (2D) material.^{1,2} Examples of such devices include graphene-insulator-graphene junctions, in which resonant peaks in the current and strong negative-differential-resistance are observed.^{1,2} Additionally, recent devices involving transition metal dichalcogenide (TMD) materials have been investigated, in which case the goal of the devices is to achieve a subthreshold swing of less than 60 mV/decade for the TFET operation.^{3,4,5}

In this work, we examine two topics, one based on theoretical prediction and the other based on experimental observation, that impact the performance of interlayer TFETs. The first topic deals with the maximum current that can be expected to be possible in such devices. An ON current of 200 μA per μm of channel width would permit the devices to be viable replacements for transistors in advanced Si technology.⁵ Theoretical predictions of current magnitudes as large as this have been made, but experimentally observed currents are much lower. To investigate this discrepancy, a detailed comparison of theory and experiment is made. Careful analysis reveals that apparent discrepancies can be reduced to about a factor of 2, hence providing validation for the theoretical predictions of large current magnitudes.

The second topic concerns moiré (interference) patterns, as in the Figure. These form when one 2D layer is placed on top of another, due to the lattice mismatch between the layers. Energy shifts of valence and conduction band electronic states are found, depending on location within the moiré pattern. The origin of these shifts is shown to involve polarization dipoles that form between the layers. These shifts, amounting to ~ 0.3 eV, lead to the formation of quantum-confined (and spatially localized) states in the system. The impact of such band shifts and localized states may be quite detrimental to the TFET operation, including, e.g., degradation of any sub-60 mV/dec subthreshold swing.



STM image (300x300nm) of triangular island of MoS_2 on WSe_2 , showing moiré pattern in the island.

¹Britnell et al., Nat. Comm. **4**, 1794 (2013). ²Fallahazad et al., Nano Lett. **15**, 428 (2015). ³Sarkar et al., Nature **526**, 91 (2015). ⁴Yan et al., Nano Lett. **15**, 5791 (2015). ⁵Li, et al., J. Electron. Mater. **46**, 1378 (2016).

This work was supported by the Center for Low Energy Systems Technology (LEAST), one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by Microelectronics Advanced Research Corporation (MARCO) and Defense Advanced Research Projects Agency (DARPA).

Collaborators include J. Li, Y. Nie, Y. Pan, S. Fölsch, Y.-C. Lin, B. Jariwala, K. Zhang, K. Cho, J. A. Robinson.

Biography – Randall Feenstra is a Professor in the Department of Physics at Carnegie Mellon University. He received his Ph.D. degree in Applied Physics from the California Institute of Technology in 1982. Dr. Feenstra joined CMU in 1995, after spending 13 years as a Research Staff Member at the IBM Research Laboratory in Yorktown Heights, New York. Dr. Feenstra is an expert in surface science investigations of semiconductors, using scanning tunneling microscopy (STM) in particular. He is a Fellow of the American Physical Society and of the American Vacuum Society.

Highly Tunable Atomic Layer Semiconducting 2D Nanoelectromechanical Systems (NEMS)

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Atomically thin semiconducting crystals derived from new classes of layered materials have rapidly emerged to enable two-dimensional (2D) nanostructures with unusual electronic, optical, mechanical, and thermal properties. The sizable and tunable bandgaps of compound and single-element 2D semiconductors offer attractive perspectives for strong multiphysics coupling and efficient transduction across various signal domains. In this presentation, we describe our team's recent highlights on studying device physics and engineering of atomic layer semiconductors and heterostructures, toward realizing ultrasensitive transducers and ultralow-power signal processing building blocks at radio frequencies (RF).

We have studied very high frequency (VHF) 2D resonant NEMS and device arrays employing transition metal di-chalcogenides (TMDCs, particularly MoS_2 , WTe_2) [1-3] and MoS_2 -graphene heterostructures [4], black phosphorus [5,6], and hexagonal boron nitride (h-BN) [7]. We have studied NEMS fundamentals such as frequency scaling [1], multimode behavior & spatial mapping [6,7], and energy dissipation [5,8]. We have also explored technologically important aspects including nonlinearity and dynamic range (DR) [9], all-electrical, on-chip integrated signal transduction [10], electrical tuning [6,10], physical sensing toward single particles [11], and mechanical tuning at large strain limit till fracture [12]. We have demonstrated highly electrically tunable multimode 2D resonant NEMS, featuring operating frequencies to >150MHz, and unconventional tuning ranges up to >300%, and deterministically measured dynamic range, $DR \sim 70$ to 100dB and even broader, with high-precision calibration of device intrinsic noise floor and onset of nonlinearity. Ongoing studies are focused on engineering the broad DR and remarkable tunability of these atomic layer 2D NEMS, towards new functions and controls in 2D nanosystems.

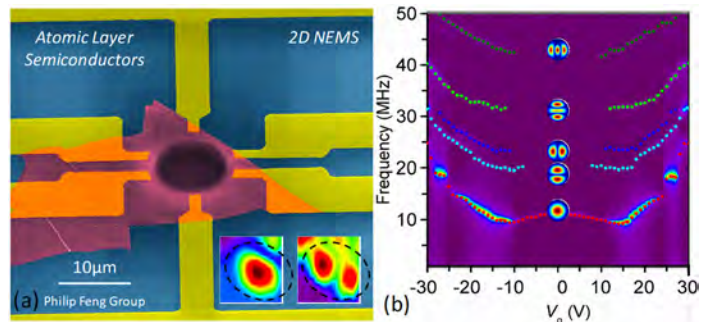


Figure 1: (a) A representative 2D NEMS device with atomic layer semiconductor in contact with 6 electrodes, suspended region being a circular drumhead. The insets (color maps of measured data) show spatially resolved resonant mode shapes. (b) Representative data exhibit the strong electrical tunability of the first 5 resonance modes.



Philip Feng is an Associate Professor in EECS at the Case School of Engineering, Case Western Reserve University (CWRU). His group's research is primarily focused on emerging semiconductor devices and integrated microsystems. He received his Ph.D. in EE from Caltech (2007). His recent awards include *NSF CAREER Award*, 4 *Best Paper Awards* (with his advisees, at *IEEE* and *American Vacuum Society* conferences), and a university-wide *T. Keith Glennan Fellowship*. He is also the recipient of the Case School of Engineering *Graduate Teaching Award* (2014) and the Case School of Engineering *Research Award* (2015). He was one of the 81 young engineers selected to participate in the *National Academy of Engineering (NAE) 2013 U.S. Frontier of Engineering (USFOE) Symposium*. Subsequently, he was selected to receive the *NAE Grainger Foundation Frontiers of Engineering (FOE) Award* in 2014. He was nominated for the *John S. Diekhoff Award* (2016) for distinguished graduate student mentoring, and for the *Bruce Jackson Award* (2016) for excellent undergraduate mentoring. Feng has >100 peer-reviewed publications and 6 patents. A Senior Member of *IEEE*, he has served on the Technical Program Committees (TPC) and as Track/Session Chairs for *IEEE IEDM*, *IEEE MEMS*, *Transducers*, *IEEE IFCS*, *IEEE SENSORS*, *IEEE NANO*, etc.

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Light Scattering and Emission from Hetero-structures

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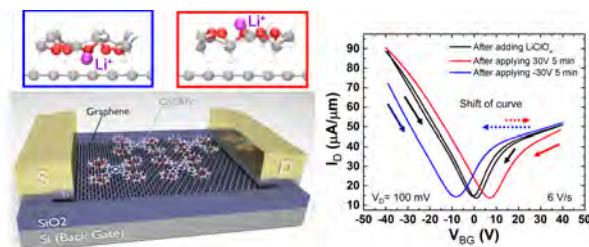
Heterostructures based on layers of atomic crystals have a number of properties often unique and very different from those of their individual constituents and of their three dimensional counterparts. The combinations of such crystals in stacks can be used to design the functionalities of such heterostructures. I will show how Raman spectroscopy can be used to fingerprint such heterostructures, and how these can be exploited in novel light emitting devices, such as single photon emitters, and tuneable light emitting diodes.

Monolayer Solid State Electrolyte for Electric Double Layer Gating of 2D Field Effect Transistors

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3. Dept. of Materials Science and Engineering, University of Texas at Dallas, Richardson TX
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A new type of solid state electrolyte is introduced for the electrostatic doping of 2D crystals using ions. The electrolyte is cobalt crown ether phthalocyanine (CoCrPc) plus a salt, which can be deposited on a 2D surface simply by drop casting and annealing. The crown ethers solvate metal ions, and hence pass through the cavity of the



crowns. The electrolyte is a single monolayer thick and arranges into a flat, ordered array. When the ions are near the surface of the channel, they induce a negative charge in the channel and hence give the low resistance, or ON state. When the ions are pushed away from the channel by an applied field, the device is in the high resistance or OFF state. Density functional theory (DFT) calculations show that the crown ethers present a small barrier to ion transport required for fast (nanosecond) switching, but the height of the barrier will be increased for long retention both by the image charge induced in the channel and by modulating the gate bias. We show that a graphene FET can be reconfigurably programmed by the monolayer electrolyte, achieving sheet carrier densities of 10^{12} cm^{-2} at a low lithium concentration of crown ethers to 1 Li^+ . Based on the geometric packing of the molecules, as determined by scanning tunneling microscopy, the doping density is predicted to increase to 10^{13} cm^{-2} at a crown ether to lithium ratio of 1:1. State retention measurements show that the two states can be retained for at least 30 minutes (maximum time measured) with a memory window of $10 \mu\text{A}$. Similar characteristics are observed for MoS_2 FETs with a larger ON/OFF ratio.

Relevant publications: Xu, K. *et al.*, **ACS Nano**, 11 (6), 5453–5464 (2017); Li, H. *et al.* **J. Phys. Chem. C**, 121, 16996–17004 (2017); Wang, W.H. *et al.*, **Solid State Ionics** 301, 176–181 (2017); Fullerton, S. *et al.*, **J. Phys. Chem. C**, 119, 21992–22000 (2015).

This work was supported in part by the Center for Low Energy Systems Technology (LEAST), one of six SRC STARnet Centers, sponsored by MARCO and DARPA, and NSF grant #ECCS GOALI 1408425.



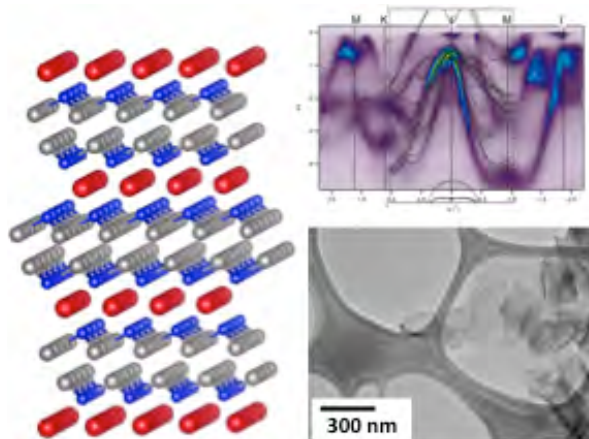
Bio: Susan Fullerton is an Assistant Professor in the Department of Chemical and Petroleum Engineering at the University of Pittsburgh. She earned her Ph.D. in Chemical Engineering at Penn State in 2009 and joined the Department of Electrical Engineering at the University of Notre Dame as a Research Assistant Professor (2009 – 2015). At Notre Dame and Pitt, she has extended her Ph.D. work on polymer electrolytes for energy storage to include applications in nanoelectronics based on 2D crystals. During the spring of 2016, Fullerton was named an ORAU Ralph E. Powe Jr. Faculty award winner. For more information: <http://fullertonlab.pitt.edu>

Tailoring Electronic and Magnetic Phenomena in New Germanium- and Tin-Containing 2D Materials

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The group 14 graphane analogues represent a unique class of covalently modifiable 2D materials, as there have been many recent exciting predictions of the existence of 2D quantum spin Hall behavior at room temperature in these materials. Inspired by these predictions, we will describe our recent efforts in the creation and properties of Ge- and Sn-containing graphane analogues, as well as new families of exfoliable Ge and Sn-containing layered Zintl phases. First, through the synthesis and characterization of a wide array of ligand-terminated germanane analogues, we have established how to rationally manipulate the electronic structure via covalent surface chemistry. Second, we will discuss our progress on developing Sn-containing graphane materials that span from trivial insulators to potentially 2D topological phases. Finally, we will discuss the synthesis and properties of new exfoliable Sn-containing layered Zintl phases, including NaSn_2As_2 and EuSn_2As_2 , which have unique anisotropic electrothermal and magnetic properties, respectively.



Josh Goldberger received his B.S. in chemistry from The Ohio State University in 2001. He received his Ph.D. in chemistry from the University of California at Berkeley in 2006, as an NSF graduate fellow. He then did his postdoctoral research at Northwestern University as part of the Institute for BioNanotechnology in Medicine, as an NIH-NRSA post-doctoral fellow (2007-2010). He has received many awards, including an MRS Graduate Student Finalist Award in 2003, an IUPAC Prize for Young Chemists in 2007, and a Camille Dreyfus Teacher-Scholar Award in 2015. He joined The Ohio State University Chemistry Department in August of 2010, and was promoted to Associate Professor in 2016. His current research interests involve designing new materials with revolutionary properties including single-atom thick 2D materials, solution-phase routes towards carbide materials, catalysts, and self-assembling peptide amphiphile based diagnostic and therapeutic agents.

GFET for high frequency applications: Impact of process on high frequency noise

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M. Deng, S. Fregonese, T. Zimmer
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Graphene and 2D materials have generated considerable interest in physics and electronic applications. Significant progresses have been made today in the field of graphene high frequency devices such as graphene field effect transistors (GFETs). Based on the state of the art, these devices can reach impressive high frequency performances. Prototypes of circuits like frequency doubler, mixers or voltage amplifiers have been demonstrated. Unfortunately, very limited works have been done on low noise amplifier (LNA) circuits, while they are the key elements for RF analogue circuits. In order to build LNA, accurate high frequency noise characterization of GFETs is of utmost importance.

In our recent work, we have studied the impact of fabrication process on noise performance of GFET. Indeed, comparing GFET with other conventional FET devices, one can observed that (i) the ratio of G_m/G_d is high due to the fact that current saturation is not easy to achieved with graphene devices, (ii) the contact resistance can be high depending of the process used, and these effects have a negative impact on noise performance. The noise performance here are measured by the method of 50Ω generator impedance (NF50), associated to a model based on small signal equivalent circuit, to extract all the noise parameters. An example of result is illustrated on Fig 1, where the four noise parameters of a back gated GFET are measured in the frequency range from 2 to 18 GHz.

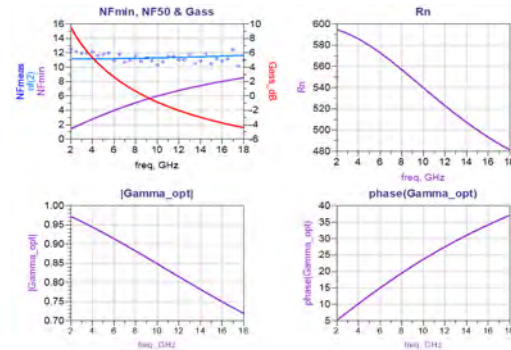


Fig. 1 : : Extraction of the four noise parameters (NFmin, Rn, Γ_{opt}) from NF50 measurement



Henri Happy received the Ph.D. degree in Electrical Engineering from the University of Lille 1, in 1992. In 1988 he joined the Institute of Electronic, Microelectronic and Nanotechnology (IEMN), one of the Lab of University Lille 1, where he is currently Full Professor of Electronics. His primary research interests are in high electron-mobility transistor (HEMT) modeling. From 1998 to 2003, his research areas were involved with the design, fabrication and characterization (up to 220 GHz) of MMICs for optical communications systems. Since 2004, his research area has focused on nanodevices, and particularly carbon devices (carbon nanotube, graphene). These activities concern understanding of fundamental limitations and improvement of

high frequency performance of carbon devices, and their applications in emerging fields of RF circuits on flexible substrates. This includes graphene growth either on SiC and metal substrate, fabrication and characterization of graphene FET. He is a leading investigator on the high frequency device research carried out under the European Graphene Flagship program. His experience is recognized by the community: he has presented many invited talks, seminars and tutorials. Henri Happy has authored or co-authored about 100 international publications and communications.

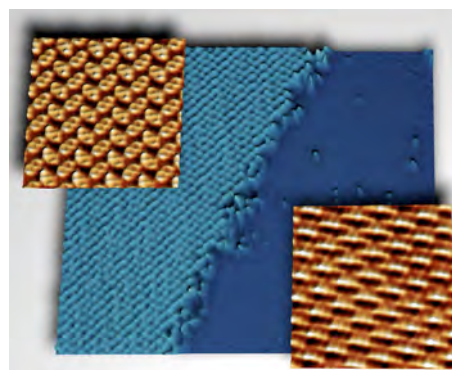
Interfacial Engineering of Two-Dimensional Nanoelectronic Heterostructures

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Two-dimensional (2D) materials have emerged as promising candidates for next-generation nanoelectronic applications [1]. With electronic properties spanning the spectrum from insulating (e.g., hexagonal boron nitride and montmorillonite) to semiconducting (e.g., transition metal dichalcogenides and phosphorene) to conducting (e.g., graphene and borophene), nearly any electronic device can be fabricated by stacking 2D materials into van der Waals heterostructures [2]. However, in the atomically thin limit, the influence of surface chemistry, defects, interfaces, and the surrounding environment often play a dominant role, especially in comparison to bulk materials [3]. Consequently, methods for controlling and characterizing heterostructure interfaces with atomic precision are critical steps towards realizing the full potential of 2D materials [4]. Towards this end, this talk will outline our latest efforts to engineer surfaces and interfaces in 2D heterostructures. For example, rotationally commensurate growth of MoS₂ has been realized on epitaxial graphene on SiC substrates [5], which allows deterministic control over grain boundary orientation [6]. For chemically reactive 2D materials (e.g., phosphorene), encapsulation with atomic layer deposition [7] and passivation with organic adlayers [8] minimize ambient degradation and provide charge transfer doping. Finally, this talk will describe emerging efforts on the growth [9,10] and chemical functionalization [11] of synthetic 2D materials (e.g., borophene) that do not exist as layered materials in the bulk.

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UHV STM image of a self-assembled borophene-organic 2D lateral heterostructure [11].



Mark C. Hersam is the Walter P. Murphy Professor of Materials Science and Engineering and Director of the Materials Research Center at Northwestern University. He also holds faculty appointments in the Departments of Chemistry, Applied Physics, Medicine, and Electrical Engineering and Computer Science. He earned a B.S. in Electrical Engineering from the University of Illinois at Urbana-Champaign (UIUC) in 1996, M.Phil. in Physics from the University of Cambridge (UK) in 1997, and a Ph.D. in Electrical Engineering from UIUC in 2000. His research interests include nanofabrication, scanning probe microscopy, semiconductor surfaces, and nanoelectronic materials. Dr. Hersam has received several honors including the Presidential Early Career Award for Scientists and Engineers, TMS Robert Lansing Hardy Award, AVS Peter Mark Award, MRS Outstanding Young Investigator, U.S. Science Envoy, MacArthur Fellowship, and seven Teacher of the Year Awards. Dr. Hersam is the co-founder of NanoIntegrus, which is a commercial supplier of nanoelectronic materials. Dr. Hersam is a Fellow of MRS, AVS, APS, AAAS, SPIE, and IEEE, and also serves as an Associate Editor of *ACS Nano*.

Back-End-of-Line Compatible WSe₂ FETs Grown by MBE on ALD Oxides

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WSe₂ grown by molecular beam epitaxy (MBE) on atomic layer deposited (ALD) high-k oxides on a Si platform is demonstrated in field-effect transistors (FETs, Figure 1a and 1b) with back-end-of-line (BEOL) compatible fabrication temperatures (< 550 °C). Using electric double layer (EDL) gating, devices exhibiting ambipolar behavior with drain currents exceeding 1 μA/μm and ON-OFF ratios greater than 10⁴ are shown in Figure 1c. Field effect hole mobilities greater than 40 cm²/V-s are measured, Figure 1d, which is orders of magnitude higher than other MBE reported TMD mobilities. The achievement of relatively high-mobility transistor channels at BEOL compatible processing temperatures shows the potential for integrating transition metal dichalcogenides (TMDs) into CMOS process flows.

This work is supported in part by the Center for Low Energy Systems Technology (LEAST), one of six centers supported by the STARnet phase of the Focus Center Research Program (FCRP), a Semiconductor Research Corporation program sponsored by MARCO and DARPA. It is also supported by the SWAN Center, a SRC center sponsored by the Nanoelectronics Research Initiative and NIST.

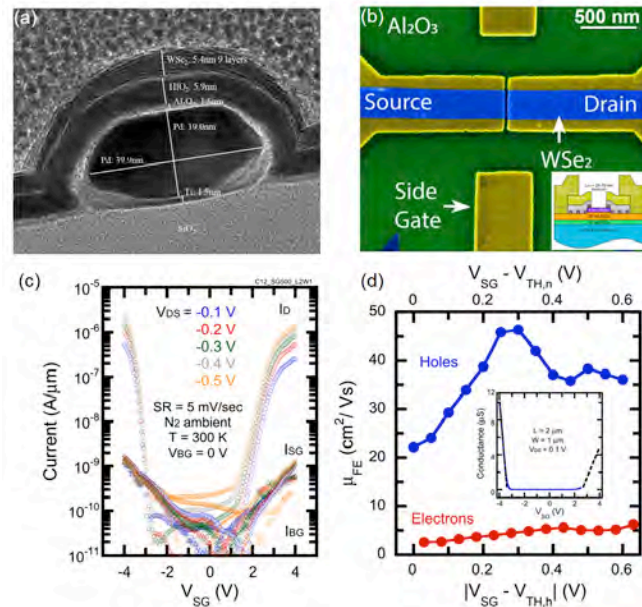


Figure 1. a) TEM of surround-channel FET with MBE-grown WSe₂, b) SEM of short-channel FET with EDL gating of WSe₂ grown on ALD Al₂O₃, c) transfer curve for the fabricated EDL-FETs, d) extracted electron and hole mobility for the EDL-FETs, with the highest reported hole mobility of MBE-grown TMDs.

Christopher Hinkle is an Associate Professor of Materials Science and Engineering at the University of Texas at Dallas, joining the faculty in the fall of 2009. He received his Ph.D. degree in 2005 in physics from North Carolina State University. Dr. Hinkle's expertise focuses on the growth, characterization, and device physics of semiconductor materials and interfaces for use in a wide variety of devices. He is particularly interested in the heterogeneous integration of two-dimensional materials, topological insulators, and III-Vs for applications related to advanced CMOS and power devices, energy harvesting, and energy storage. He has authored or co-authored over 95 publications in peer-reviewed journals and presented more than 65 contributed and 35 invited talks at international meetings. He is a member of numerous professional organizations including APS, AVS, ECS, IEEE, and MRS.

Dynamic Rotational Control of van der Waals Heterostructures

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Electronic, mechanical, and vibrational properties of layered van der Waals heterostructures can be highly dependent on the relative crystallographic orientation between the layers. However, control over this parameter has been insufficient to date. We achieve dynamic angular control between two atomically flat layered materials by physically pushing the uppermost section of the heterostructure with an atomic force microscope (AFM) in contact mode. In this way, we can adjust the interlayer rotation angle by steps as small as 0.1° , and measure continuous variation in properties with angle within the same sample. In the first studies using this technique, we have focused on heterostructures of graphene and hBN, where the rotational angle changes the wavelength of the moire' pattern between the two lattices. We are able to measure changes in the electronic bandstructure, including the position and magnitude of moire'-induced bandgaps, with angle. We simultaneously measure the Raman linewidth with angle and find agreement with previous studies, but with reduced experimental scatter. Finally, we observe that the interlayer friction strongly increases with crystallographic alignment.

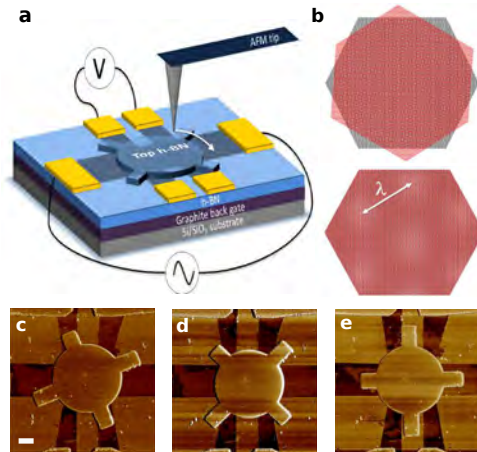


Figure 1. (a) schematic of AFM rotation of vdW heterostructure. (b) Moire' patterns for hBN and graphene. (c-e) AFM images of rotating structure



James Hone is currently Wang Fong-Jen Professor of Mechanical Engineering at Columbia University, and director of PAS³, Columbia's Materials Science Research and Engineering Center (MRSEC). He received his PhD in experimental condensed matter physics from UC Berkeley in 1998, and did postdoctoral work at the University of Pennsylvania and Caltech, where he was a Millikan Fellow. He joined the Columbia faculty in 2003. His current research interests include synthesis, characterization, manipulation, and applications graphene, and other 2D materials; nanomechanical devices; and nano-biology.

Toward 2D-CMOS Integration

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Two-dimensional (2D) atomic-layer materials such as graphene, molybdenum disulfide (MoS_2), and black phosphorus are promising materials for future-generation flexible and high-speed electronics that can operate efficiently at gigahertz and terahertz frequencies, respectively. However, the world is three dimensional and it will be difficult for 2D materials to stand on their own. Further, to date most 2D devices are individually crafted on small exfoliated flakes using direct-write electron-beam lithography, which is not suitable for large-scale integration and manufacturing. To effectively interface 2D materials with the real world, it will be desirable to integrate them with state-of-the-art complementary metal-oxide semiconductor (CMOS) technology, using its well-developed batch process with silicon substrate and stepper photolithography. Toward this end, we report the first batch processing by stepper photo lithography of thousands of MoS_2 MOS field-effect transistors (FETs) with submicron gate length, -3.0 ± 1.6 V threshold, and over 50% yield (Fig. 1). More details of the preparation of large-area 2D materials, the challenge in patterning fragile 2D materials, and their implication for the future of 2D materials and devices will be discussed.

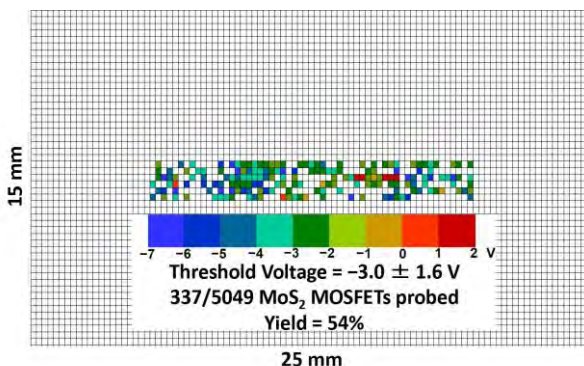


Fig. 1. Wafer map of mono-layer MoS_2 MOSFET with 0.2 μm gate length and 10 μm gate width.

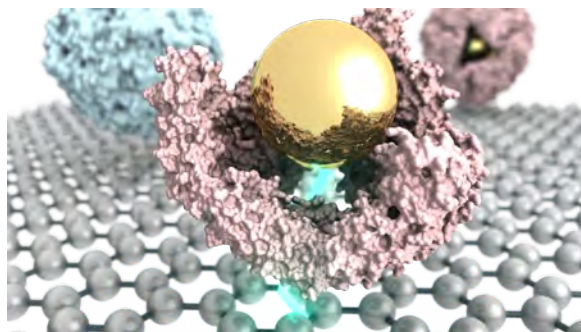


Dr. James Hwang is Professor of Electrical Engineering at Lehigh University. He graduated with a B.S. degree in Physics from National Taiwan University, and M.S. and Ph.D. degrees in Materials Science from Cornell University. After twelve years of industrial experience at IBM, Bell Labs, GE, and GAIN, he joined Lehigh in 1988. He cofounded GAIN and QED; the latter became a public company (IQE). He has been a visiting professor at Shanghai Jiao Tong University, East China Normal University, and University of Science and Technology in China, Nanyang Technological University in Singapore, and Marche Polytechnic University in Italy. Most recently, he was a Program Officer for GHz-THz Electronics at the US Air Force Office of Scientific Research. He is a Life Fellow of the Institute of Electrical and Electronic Engineers. He has published more than 300 refereed technical papers with the impact factor $h > 40$ according to Google Scholar. He has been granted eight U. S. patents. He has researched on the design, modeling and characterization of microwave, optical and micro-electromechanical (MEM) devices and integrated circuits. His current research interest focuses on radio-frequency MEM systems, electromagnetic sensors for individual biological cells, two-dimensional atomic layered materials and devices, and scanning microwave microscopy.

"Beyond" Graphene Bio-Nano Hybrids for Programmable Chemical Detection

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Two-dimensional materials (sometimes called “atomic layer materials”) have emerged as a scientific playground for the exploration of new phenomena, with numerous potential applications already demonstrated and proposed. I will discuss our work on large-area growth methods for monolayer materials, including graphene, boron nitride, and the rich materials family known as transition metal dichalcogenides (TMDs). Of particular interest is our recent progress in chemical vapor deposition of monolayer MoTe₂ and WTe₂ in the 1T' structure, both predicted to host topological electronic states. Along with the basic science of the materials, we have explored all-electronic chemical detectors based on bio-nano hybrids, where a biomolecule provides chemical recognition and a graphene or monolayer molybdenum disulfide (MoS₂) transistor enables electronic readout. Capitalizing on rapid advances in 2D materials research and biomolecular engineering, this sensor class represents a promising approach towards sensitive and selective detection of liquid- and vapor-phase analytes. Such bio-nano hybrids enable detection of protein cancer biomarkers, antigen from various pathogens, small molecule targets, and nucleic acid oligomers at femtomolar concentrations and below. Related methods can be used to create all-electronic vapor sensors that are able to discriminate between highly similar compounds such as enantiomers and very similar complex vapor mixtures characteristic of humans. Recently we have shown the promise of this system for diagnosis of disease based on volatile biomarkers.



A.T. Charlie Johnson is a Professor of Physics at the University of Pennsylvania. He received a BS from Stanford University, and MS and PhD from Harvard University, all in Physics. He was a European Union ESPRIT Postdoctoral Fellow at the Delft University of Technology and a National Research Council Postdoctoral Research Fellow at the National Institute of Standards and Technology. His research group is focused on nanostructure physics and nanoelectronics, with interests in the science and applications of carbon nanotubes, graphene, and other two-dimensional materials. Johnson's honors include a NSF Graduate Research Fellowship, a Packard Science and Engineering Fellowship, a Sloan Fellowship, and selection as a Fellow of the American Physical Society and the American Association for the Advancement of Science. He is also a member of the Defense Science Study Group (2018-19). Johnson has authored over 200 peer-reviewed articles and holds 12 awarded patents, with 10 other patents submitted. He is a member of the Founding Editorial Board of AIP Advances and Co-Founding Scientist of Graphene Frontiers.

Van der Waals Solids: Enabling Advances in Printed Electronics and Photosensing Applications

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Abstract: Two-dimensional (2D) layered nanomaterials such as graphene, black phosphorus and transition-metal dichalcogenides (TMDCs) have attracted tremendous attention over recent years due to their unique properties and potential for numerous applications. Top-down synthesis of these materials utilize solution-based chemical exfoliation to form inks which are printed using additive manufacturing techniques in a printed electronics platform to form devices. The devices range from high-power resistors, capacitors and photodetectors. In particular, an inkjet printed, biocompatible, heterostructure photodetector was constructed using inks of photo-active molybdenum disulfide (MoS_2) and electrically conducting graphene which facilitated charge collection of the photocarriers, where the heterojunction devices were responsive to broadband incoming radiation in the visible regime. Our efforts in the bottom-up synthesis of these materials using chemical vapor deposition (CVD) with oxide precursors shows we form binary compounds of sulphides and selenides that are characterized using Raman Spectroscopy, Photoluminescence and Atomic Force Microscopy, which we implement for photodetectors, solar cells, and other related applications.



Bio: Anupama B. Kaul is the PACCAR Endowed Professor of Engineering and serves as Director of the PACCAR Technology Institute at the University of North Texas (UNT), where she started her appointment in September, 2017. At UNT she is with the Department of Materials Science and Engineering and holds a joint appointment in the Department of Electrical Engineering. Prior to UNT, Prof. Kaul served as the Associate Dean for Research and Graduate Studies in the College of Engineering at the University of Texas, El Paso (UTEP) and held The AT&T Distinguished Professorship in the Department of Electrical and Computer Engineering. Her research lab is comprised of the 1) Electronics and Opto-electronics Materials and Device Characterization Lab; and the 2) Materials Synthesis, Composites and Bio-materials Processing Lab. Prior to UTEP, Prof. Kaul served as a Program Director at the National Science Foundation (NSF) in the Engineering Directorate from 2011-2014. Prof. Kaul's NSF appointment was through the IPA program with the Jet Propulsion Laboratory (JPL), California Institute of Technology (Caltech) where she spent a total of 12 years. She obtained her M.S. and Ph.D. degrees from the University of California, Berkeley in Materials Science and Engineering with minors in Electrical Engineering and Physics. She is the recipient of the National Science Foundation's Director's Award for Program Management Excellence in 2013. At JPL-Caltech, Prof. Kaul received the NASA Service Award, a NASA Team Accomplishment Award, multiple NASA Patent Awards and numerous NASA Technology Brief Awards for her research. In 2012, Prof. Kaul was selected to be a participant at the US National Academy of Engineering (NAE) Frontiers of Engineering (FOE) Symposium, and in 2014 she was invited to participate in the bi-lateral Indo-US FOE, also organized by the US NAE.

Commensuration and Incommensuration in the van der Waals Heterojunctions

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Heterogeneous interfaces between two dissimilar materials are an essential building block for modern semiconductor devices. The 2-dimensional (2D) van der Waals (vdW) materials and their heterostructures provide a new opportunity to realize atomically sharp interfaces in the ultimate quantum limit for the electronic and optoelectronic processes. By assembling atomic layers of vdW materials, such as hexa boronitride, transition metal chalcogenide and graphene, we can construct atomically thin novel quantum structures. We demonstrate the enhanced electronic and optoelectronic performances in the vdW heterostructures, suggesting that these a few atom thick interfaces may provide a fundamental platform to realize novel physical

phenomena. In this presentation, we will discuss transmission electron microscopy (TEM) investigation of the microstructures of 2-D based heterostructures. Microstructural properties of the heterostructures caused by the interlayer interaction were studied by TEM-based analytical techniques such as electron diffraction, dark field imaging, and aberration corrected scanning TEM imaging. We show that the commensurate domain structures can be formed as a result of the interplay between van der Waals interaction energy and elastic energy of individual layers. Based on the experimental data, we identify microstructural origin that can cause the structural transition in the system.

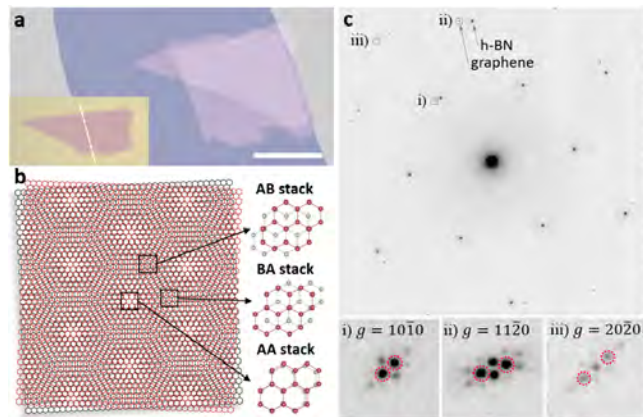


Fig. 1a. False-color optical microscope image of artificial bilayer graphene with controlled twist angle covered with h-BN layer. b. Schematic diagram of twisted bilayer graphene without any reconstruction. c. SAED pattern of twisted bilayer graphene covered with h-BN layer.



Professor Philip Kim received his Ph. D. in Applied Physics from Harvard University in 1999. He was Miller Postdoctoral Fellow in Physics from University of California, Berkeley during 1999-2001. He then joined in Department of Physics at Columbia University as a faculty member during 2002-2014. Since 2014, he moves to Harvard University, where he is Professor of Physics and Professor Applied Physics. The focus of Prof. Kim's group research is the mesoscopic investigation of transport phenomena, particularly, electric, thermal and thermoelectrical properties of low dimensional nanoscale materials. Professor Kim published more than 180 papers in professional journals which are well cited. Professor Kim also received numerous honors and award including Oliver E. Buckley Prize (2014), Dresden Barkhausen Award (2011); IBM Faculty Award (2009); and Ho-Am Science Prize (2008). In addition, He has given more than 300 invited presentations as keynote speaker, plenary speakers, and invited speakers in international and domestic conferences, colloquiums and department seminars.

Graphene Flagship: the present status and future plans

Jari Kinaret

Department of Physics

Chalmers University of Technology

SE-41296 Gothenburg, Sweden

In this talk I will briefly discuss the Graphene Flagship, its past, present and future. I will focus on the flagship in the global context, and will not cover the details of our scientific and technological work – they will be discussed by other workshop participants.



Jari Kinaret received his M.Sc. degrees in Theoretical Physics and Electrical Engineering at the University of Oulu, Finland, in 1986 and 1987, respectively, and in 1992 he graduated with Ph.D. in Physics from the Massachusetts Institute of Technology. After a brief stay in Copenhagen, he moved to Sweden in 1995 where he works as a Professor of Physics at the Chalmers University of Technology. His research is theoretical condensed matter physics, and his main interests in the last years have been nanoelectromechanical systems as well as optical properties of graphene. He has been the driving force behind the research initiative Graphene Flagship since 2010, and is the Director of this one billion euro endeavor since the project start in 2013.

Valley/spin devices based on 2D TMDCs

Andras Kis

EPFL, Lausanne, Switzerland

The band structure of transition metal dichalcogenides (TMDCs) with valence band edges at different locations in the momentum space could be harnessed to build devices with operation relying on the valley degree of freedom. To realize such valleytronic devices, it is necessary to control and manipulate the charge density in these valleys. In my talk, I will present our recent efforts in this direction. In the first part, I will present our demonstration of spin injection from a ferromagnetic electrode into a TMDC-based heterojunction. In the second, I will present how by relying the valley/spin degree of freedom in TMDC we can optically inject spin into a WSe₂/graphene heterostructure and detect the resulting spin current in graphene using ferromagnetic electrodes.

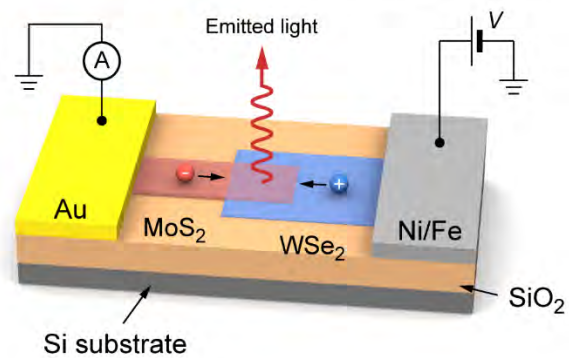


Figure 1. Valley/spin LED based on a dichalcogenide heterostructure.



Dr. Andras Kis is a Professor of Electrical Engineering and Materials Science at EPFL, Lausanne. His research is focused on the fundamental science and device applications of 2D semiconductors. Prior to joining EPFL as faculty, he was a postdoctoral researcher at UC Berkeley in the group of Alex Zettl, where he studied electrical and mechanical properties of carbon and boron nitride nanotubes. He received his Ph.D. in physics from EPFL in 2003 and received his MSc in physics from the University of Zagreb, Croatia. His papers have received more than 21000 citations with the h factor >46 according to Google Scholar. His major awards include the Latsis prize in 2004, ERC starting grant in 2009 and ERC consolidator grant in 2015, both awarded for research in the area of 2D transition metal dichalcogenides. Andras Kis is also serving as the editor-in-chief of the Nature partner journal, NPJ 2D Materials and Applications.

Graphene CMOS camera for visible and infrared light

Frank Koppens

The Institute of Photonics Sciences (ICFO), Barcelona, Spain

ICREA – Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain.

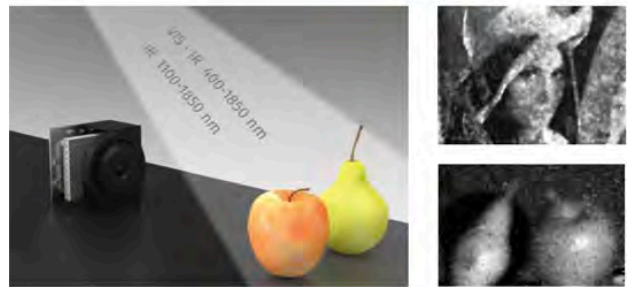
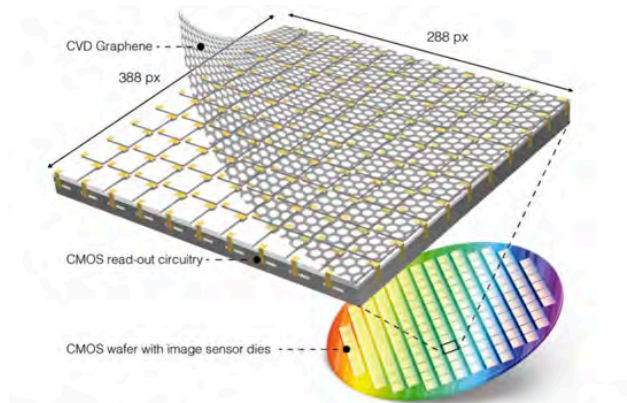
Integrated circuits based on CMOS (complementary metal-oxide semiconductors) are at the heart of the technological revolution of the past 40 years, as these have enabled compact and low cost micro-electronic circuits and imaging systems. However, the diversification of this platform into applications other than microcircuits and visible light cameras has been impeded by the difficulty to combine other semiconductors than silicon with CMOS.

We show for the first time the monolithic integration of a CMOS integrated circuit with graphene as a high-resolution image sensor and operate it as a digital camera for visible and infrared light at the same time. We integrated graphene and the image sensor read-out circuit with a pixel yield of 99.8%. Subsequently the graphene was coated with a layer of colloidal quantum dots to sensitize it to UV, visible and infrared light (300 – 2000 nm) [2, 3]. Applications for automotive, night vision, food inspection, medical imaging have been demonstrated.

[1] Goossens et al., *Nature Photonics* (2017).

[2] G. Konstantatos, et al., *Nature Nanotechnology* 7, 6, 363 (2012).

[3] Nikitskiy et al., *Nat. Communications* 7 (2016).



Prof. Frank Koppens obtained his PhD in experimental physics at Delft University, at the Kavli Institute of Nanoscience, The Netherlands. After a postdoctoral fellowship at Harvard University, since August 2010, Koppens is a group leader at the Institute of Photonic Sciences (ICFO). The quantum nano-optoelectronics group of Prof. Koppens focuses on both science and technology of novel two-dimensional materials and quantum materials. Koppens has received four ERC grants, the Christiaan Huygensprijs 2012, the national award for research in Spain, and the IUPAP young scientist prize in optics. Prof. Koppens is leader of the optoelectronics workpackage of the graphene flagship (1B€ project for 10 years). In total, Koppens has published more than 70 refereed papers (H-index 38), with more than 30 in Science and Nature family journals. Total citations >10.000.

Synthesis and Characterization of Mixed-Dimensional Heterostructures

Michael Moody¹, Alexander Henning¹, Jack Olding², Ju-Ying Shang¹, Jade Itamar-Balla¹, Zhiyuan Sun¹, Mark C. Hersam^{1,2,3}, Emily Weiss^{1,2,3}, and Lincoln J. Lauhon¹

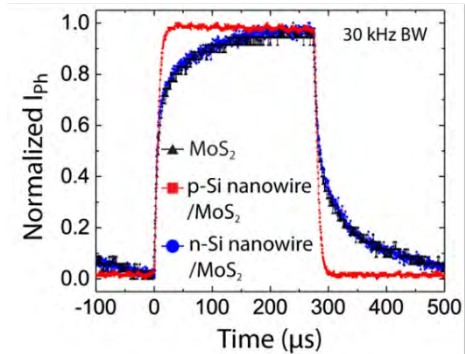
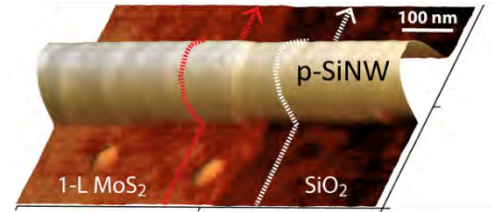
¹Department of Materials Science and Engineering

²Department of Chemistry and Chemical Biology

³Applied Physics Program

Northwestern University, Evanston, IL

The exposed interfaces of two-dimensional (2D) materials provide a wealth of opportunities to engineer their properties and build new types of heterojunctions, but scalable fabrication of materials with controlled properties remains a challenge. We have used a combination of atomic layer deposition and microfabrication to integrate metal dichalcogenides into new 0D-2D and 1D-2D heterostructures in which the geometry influences fundamental properties and device performance. Control of carrier concentration through extrinsic doping and gating through a dielectric are foundations of device engineering. We have used atomic layer deposition (ALD) of MoO_x on MoS_2 to provide environmental isolation and controlled doping through variation in the oxidation state of the dielectric. Shifts in work function are well correlated with deposition conditions and device behaviors. ALD was also used to grow 0D-2D and 2D-2D van der Waals heterostructures through controlled nucleation and step-edge growth; intentional modifications of surface chemistry are shown to strongly influence nucleation behaviors. Finally, 1D-2D *p-n* heterostructures (see figure above) were explored through direct transfer of 2D MoS_2 on p-type Si nanowires. Scanning probe characterization and device modeling are used to extract materials parameters and device operating principles for benchmarking against conventional heterostructures. The fast photoresponse of 1D-2D *p-n* junctions is shown to arise from the depletion region in the 2D material, and the benefits of using multilayer rather than monolayer 2D materials are evaluated.



Prof. Lauhon is a Professor and Associate Chair in the Department of Materials Science and Engineering at Northwestern University and Co-Director of the Applied Physics Program. He received a Ph.D. in Physics from Cornell with Wilson Ho (2000) and a B.S. in Physics from the University of Michigan (1993). Prior to joining Northwestern in 2003, he was a postdoctoral researcher in the Department of Chemistry and Chemical Biology at Harvard University with Charles Lieber. At Northwestern, the Lauhon group investigates novel structure-property relationships in nanostructured materials and heterostructures using correlated imaging methods that probe structure, composition, and function. His work has been recognized with an NSF CAREER Award, a Sloan Fellowship in Chemistry, and a Camille Dreyfus Teacher Scholar Award. He is the author of over 140 refereed papers with an H-index of 46. In collaborative endeavors, he leads IRG-1 in the Northwestern University MRSEC, and serves on the Board of Directors for the Materials Research Society.

Correlated Nanoelectronics

Jeremy Levy^{1,2}

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The study of strongly correlated electronic systems and the development of quantum transport in nanoelectronic devices have followed distinct, mostly non-overlapping paths. Electronic correlations of complex materials lead to emergent properties such as superconductivity, magnetism, and Mott insulator phases. Nanoelectronics generally starts with far simpler materials (e.g., carbon-based or semiconductors) and derives functionality from doping and spatial confinement to two or fewer spatial dimensions. In the last decade, these two fields have begun to overlap. The development of new growth techniques for complex oxides have enabled new families of heterostructures which can be electrostatically gated between insulating, ferromagnetic, conducting and superconducting phases. In my own research, we use a scanning probe to “write” and “erase” conducting nanostructures at the $\text{LaAlO}_3/\text{SrTiO}_3$ interface. The process is similar to that of an Etch-a-Sketch toy, but with a precision of two nanometers. A wide variety of nanoscale devices have already been demonstrated, including nanowires, nanoscale photodetectors, THz emitters and detectors, tunnel junctions, diodes, field-effect transistors, single-electron transistors, superconducting nanostructures and ballistic electron waveguides. These building blocks may form the basis for novel technologies, including a platform for complex-oxide-based quantum computation and quantum simulation.



Dr. Jeremy Levy is a Distinguished Professor of Condensed Matter Physics at the University of Pittsburgh in the Department of Physics and Astronomy (<http://levylab.org>), and Founding Director of the Pittsburgh Quantum Institute (<http://pqj.org>). He received an A.B. degree in physics from Harvard University in 1988, and a Ph.D. degree in physics from UC Santa Barbara in 1993. After a postdoctoral position at UC Santa Barbara, he joined the University of Pittsburgh in 1996. His research interests center around the emerging field of oxide nanoelectronics, experimental and theoretical realizations for quantum computation, semiconductor and oxide spintronics, quantum transport and nanoscale optics, and dynamical phenomena in oxide materials and films. He is a Class of 2015 Vannevar Bush Faculty Fellow, a Fellow of the American Physical Society, a recipient of the 2008 Nano50 Innovator Award, and the NSF Career Award. He has received the University of Pittsburgh's Chancellor's Distinguished awards for research (2004, 2011) and teaching (2007).

Gate Induced Superconductivity in Transition Metal Dichalcogenides

Alberto F. Morpurgo

DQMP & GAP, University of Geneva,

24 quai Ernest-Ansermet, CH1211 Geneva, Switzerland.

In this talk I will present an overview of our work on gate induced superconductivity in transition metal dichalcogenides. After a short introduction about the technique of ionic liquid gating, I will discuss our observation of a gate-induced superconducting state in MoS_2 that persists even when the thickness of the material is reduced to an individual monolayer. I will summarize the key observation concerning the evolution of the superconducting properties with thickness, which are not fully understood at the moment. In the second part of the talk I will concentrate on very recent tunneling spectroscopy experiments that have allowed us to directly probe the superconducting gap as a function of carrier density. In agreement with expectations for an Ising superconducting state, we find that the density of states is not affected by applying in-plane magnetic fields as large as 10 T. We also discuss the indication given by tunneling spectroscopy as to the microscopic nature of the superconducting state and show that many of the observations point to a so-called $s\pm$ state characteristic of two-band superconductivity due to repulsive interactions (analogous to what is considered to be the state in Fe-based pnictides superconductors).

Work done in collaborations with D. Costanzo, H. Zhang, A. Reddy, S.Jo, and H. Berger



Alberto Morpurgo is a Full Professor at the University of Geneva, Switzerland. He received his Laurea degree from the University of Genova (Italy) and his PhD in Physics from the University of Groningen (the Netherlands). Before moving to Geneva, prof. Morpurgo has worked at Delft University and Stanford University. He is an expert in nanoelectronics, quantum transport, and 2D materials, has worked on a broad variety of domains including phase coherent electron transport, superconducting proximity effect, spin-orbit interaction, carbon nanotubes, topological insulators, and more. The current activity of Morpurgo's research group is mainly focusing on the study of 2D materials and their interfaces, and heavily exploits field-effect techniques –including ionic liquid gating– to

control the electronic state of these systems. Prof. Morpurgo is Deputy leader of WP1 Enabling Science and Technology of the EU Graphene Flagship, he is a member of the Research Council of the Swiss National Science Foundation, and is also member of the editorial boards of 2D Materials and Physical Review Materials.

2D nanosheet electronics and optoelectronics

T. Mueller

Vienna University of Technology, Institute of Photonics, Vienna, A-1040, Austria

The materials that have enabled the information technology revolution over the past decades will soon reach their physical limits. Novel nanomaterials and technolo-

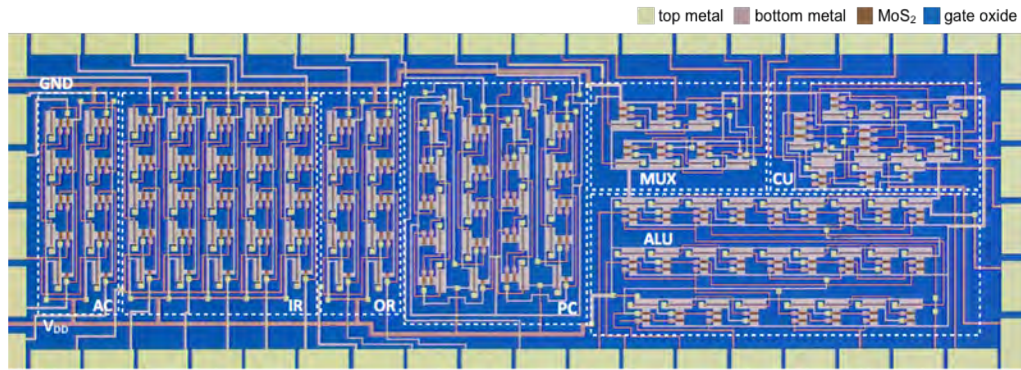


Fig. 1: Microscope image of a simple MoS₂-based 2-bit microprocessor.

gies have therefore become a major focus of current solid-state device research, with two-dimensional (2D) atomic crystals being one of the most promising candidates. Among them, transition metal dichalcogenides (TMDs) have come into the focus of interest, as these allow for the construction of logic transistors, light emitters, photovoltaic solar cells, and other electronic devices. In this talk, I will present some of our results on the development of electronic circuits based on 2D materials. Large-area MoS₂ growth, together with the development of 2D logic stages, enabled us to realize large-scale digital circuits, such as simple 1-bit and 2-bit microprocessors. In the second part of this talk I will review our recent activities on TMD optical spectroscopy and optoelectronics. In particular, a method will be presented that allows for measurements of the local strain matrix in TMDs based on optical second harmonic generation. This method relies on the strain-induced modification of the nonlinear susceptibility tensor due to the photoelastic effect. Using a two-point bending technique, we determine the photoelastic tensor elements of MoS₂. Once identified, these parameters allow us to spatially map the strain field in an inhomogeneously strained sample. Finally, I will discuss type-II TMD van der Waals heterojunctions for the realization of ultrathin photovoltaic solar cells. I will present a device model that is able to fully reproduce the current-voltage characteristics under optical illumination, including some peculiar behaviors such as exceedingly high ideality factors or bias-dependent photocurrents.



Thomas Mueller received his M.S. and Ph.D. degrees in Electrical Engineering from TU Vienna in 2001 and 2004, respectively. In 2007 he joined the IBM Watson Research Center, USA, as a Postdoc, working on carbon-based optoelectronics. At the end of 2009 he returned to TU Vienna, where he currently holds an Associate Professor position. His research focuses on electronic and optoelectronic devices based on two-dimensional materials. He (co-)authored 75 peer-reviewed publications in leading scientific journals. Selected awards include the START-Prize, the Fritz Kohlrausch-Prize, and the ASciNA Award.

From epitaxy to science and technologies of metal chalcogenide van der Waals crystals

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The development of van der Waals (vdW) heterostructures made by stacking two dimensional (2D) crystals has led to the discovery of fundamental physical phenomena and to the realization of 2D functional devices ranging from sensitive phototransistors to tunnel diodes. The electronic properties of these devices can be modified not only by careful selection of the materials within the stack, but also by adjusting the built-in strain and relative orientation of the component crystalline layers. Among the vdW crystals, the metal chalcogenide InSe compound represents an exfoliable and stable semiconductor that expands the current library of vdW crystals. In this talk I will review the research at Nottingham on this new class of 2D layered compounds. From the growth and fabrication of vdW heterostructures to the demonstration of prototype graphene/InSe devices, I will discuss how these layers can provide a platform for scientific investigations and new routes to 2D electronics and optoelectronics [1-4].

1 G.W. Mudd et al., *Advanced Materials* 25, 5714 (2013); *ibidem* 27, 3760 (2015).

2 G.W. Mudd et al., *Scientific Reports* 6, 39619 (2016).

3 D.A. Bandurin et al. *Nature Nanotechnology* 12, 223, (2017).

4 N. Balakrishnan et al. *2D Materials* 4, 25043 (2017).



Prof. Amalia Patanè studied at the University of Rome “La Sapienza” where she graduated with first-class honours in Physics in 1994 and a PhD in 1998. She has worked as a Research Associate (1998-2002) in the School of Physics and Astronomy of the University of Nottingham, where she conducted the first imaging by magneto-tunneling of electrons confined in a nanocrystal (*Science* 2000). As a lecturer at Nottingham (2002-06), she has developed further her research on quantum systems by exploring novel carrier dynamics in high magnetic fields (*Nature* 2004). She was promoted Reader in 2006 and Professor of Physics in 2011. Her current research focuses on novel van der Waals two dimensional crystals (*Nature Nanotechnology* 2017; *Physical Review Letters* 2017). Prof. Patanè leads the University of Nottingham in the EU Graphene Flagship (<http://graphene-flagship.eu/>) and as a member of the Council of the European Magnetic Field Laboratory, EMFL (<http://www.emfl.eu/home.html>), she promotes the development of high magnetic field facilities and their application to study important materials in condensed matter physics. Her research achievements were recognized by the Sir Charles Vernon Boys Medal and Prize of the Institute of Physics (2007), an EPSRC Advanced Research Fellowship (2004-09) and a Leverhulme Trust Research Fellowship (2017-19). She is also a Member of the International Union of Pure and Applied Physics Commission (IUPAP, Semiconductor Commission 2014-20) and the Council Board of the EMFL (2015-20).

Towards Low-Voltage Electronic Devices using 2D-TMD Vertical Heterostructures

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¹School of Materials Science and Engineering, Georgia Institute of Technology

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Two-dimensional (2D) transition metal dichalcogenides (TMDs) provide unique material properties that make them attractive candidates for next-generation low voltage electronics, with applications in beyond-CMOS low-power computing and large-area flexible electronics. Unlike traditional materials, where a lattice match between adjacent thin films is critical, heterogeneous 2D layers can be stacked using Van der Waal's attraction to form vertical heterostructure-based electronic devices. In this work, we first demonstrate via simulation that 2D TMD-based resonant tunneling devices can outperform III-V based equivalent devices by providing a larger peak-to-valley ratio (PVR). The developed model also enables the analysis of a 2D interlayer tunnel field-effect transistor (ITFET) with an ideal sub-threshold slope below the 60 mV/decade limit for today's Si technology. The impact of realistic device constraints, such as device size and rotational misalignment, are also taken into account. Experimental results for large-area CVD graphene-MoS₂-graphene vertical heterostructures are then presented, which shed light on the impact of direct heterostructure synthesis and consequent elemental intermixing. This motivates the development of low-temperature, plasma-assisted growth of 2D TMDs, resulting in the successful synthesis of MoS₂ at 400°C. Though characterization of these films show defect-dominated carrier transport, it is believed that further optimization and reduced growth rates can yield improved film quality. Lastly, the development of low-voltage MoS₂-based Schottky diodes for future flexible systems is presented.

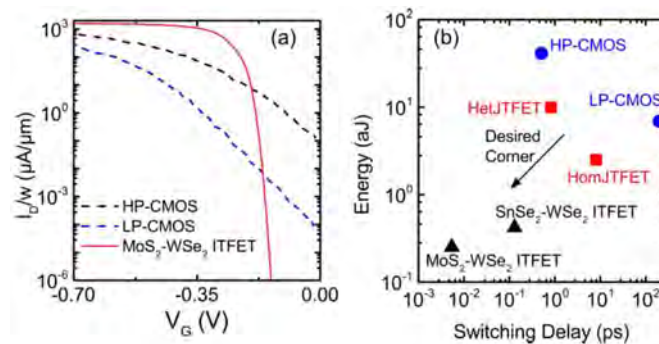


Fig. 1 (a) Comparison of the transfer curve of the MoS₂-WSe₂ ITFET with HP and LP CMOS devices. (b) Comparison of the energy and switching delay for the MoS₂-WSe₂ ITFET with tunneling devices from other technologies. [1]



Dr. Spyridon Pavlidis has been a post-doctoral fellow in the School of Materials Science and Engineering at the Georgia Institute of Technology since 2016. In January 2018, he will join the School of Electrical and Computer Engineering at North Carolina State University as an Assistant Professor. He received the M.Eng degree in Electrical and Electronic Engineering from Imperial College London in 2010, and the Ph.D. degree in Electrical and Computer Engineering from the Georgia Institute of Technology in 2016. Spyridon's research interests lie at the intersection of electronic materials, devices, packaging and circuits. In recent years, he has focused on novel 2D material devices, flexible potentiometric biosensors and high-power wide bandgap semiconductor devices. He has published more than 20 journal and conference papers in these areas.

[1] P. M. Campbell, J. K. Smith, W. J. Ready, and E. M. Vogel, "Material Constraints and Scaling of 2-D Vertical Heterostructure Interlayer Tunnel Field-Effect Transistors," *IEEE Transactions on Electron Devices*, vol. 64, no. 6, pp. 2714-2720, 2017.

Turning the electronic properties of phosphorene: straining, stacking, gating and twisting

F.M. Peeters

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Due to the strong anisotropic atomic structure of BP, its electronic conductivity and optical response are sensitive to the magnitude and the orientation of the applied strain. Applied tensile strain significantly enhance electron transport along zigzag direction of BP. Biaxial strain is able to tune the optical band gap of monolayer BP from 0.38 eV (at -8% strain) to 2.07 eV (at 5.5%). The exciton binding energy is also sensitive to the magnitude of the applied strain. It is found to be 0.40 eV for compressive biaxial strain of -8%. and it becomes 0.83 eV for tensile strain of 4%.

The effect of the number of stacking layers and the type of stacking of BP layers influences its electronic properties. Different stacking types result in similar energetics, the size of the band gap and the optical response of bilayer and trilayer phosphorene are very sensitive to the number of layers and the stacking type. Regardless of the number of layers and the type of stacking, bilayer and trilayer black phosphorus are direct band gap semiconductors whose band gaps vary within a range of 0.3 eV. Stacking arrangements that are different from the ground state structure in both bilayer and trilayer BP exhibit significant modified valence bands along the zigzag direction and result in larger hole effective masses. The optical gap of bilayer (trilayer) black phosphorus varies by 0.4 (0.6) eV when changing the stacking type. The calculated binding energy of the bound exciton hardly changes with the type of stacking and is found to be 0.44 (0.30) eV for bilayer (trilayer) phosphorous.

The electronic spectrum of 90° twisted bilayer black phosphorus is found to be x-y isotropic in contrast to the monolayer. However x-y anisotropy, and a partial return to monolayer-like behavior, particularly in the valence band, can be induced by an external out-of-plane electric field. Moreover, the preferred hole effective mass can be rotated by 90° simply by changing the direction of the applied electric field. Our simulations clearly indicate that the twist angle in combination with an appropriate gate voltage is a novel way to tune the electronic and optical properties of bilayer phosphorus and it gives us a new degree of freedom to engineer the properties of black phosphorus based devices.

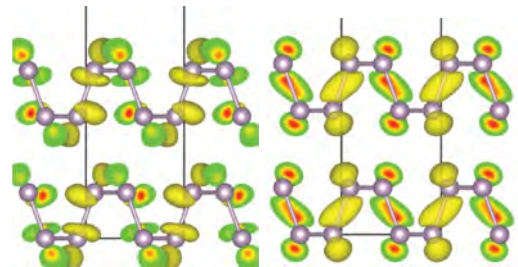


Fig.: Side view of charge density of CBM and VBM for AA stacked bilayer BP.



Dr. François Peeters is Professor of Physics at the University of Antwerp. He received the PhD degree in physics from the University of Antwerp in 1982. He did postdoctoral research at Bell Laboratory (Murray Hill, NJ, USA) and Bell Communications Research (Red Bank, NJ, USA). Peeters is a Fellow of the American Physical Society and the European Physical Society. He is a member of the Royal Flemish Academy of Belgium and of the Academia Europaea. The University of Szeged awarded him a Doctor Honoris Causa and in 2013 he was awarded the

Francqui Chair. He is associate editor of Journal of Applied Physics, co-editor of Europhysics Letters and member of the executive editorial board of Solid State Communications. He published over 1000 papers with more than 29,000 citations and h-index 77. His areas of interests are computational modelling of mesoscopic and nanoscopic semiconductor and superconducting nanostructures, like phase transitions (structural and melting), artificial atoms (quantum dots and coupled quantum dots), graphene and other two dimensional atomic layered systems.

Recent advances in the fundamental physics of graphene-based van der Waals heterostructures

Marco Polini^{1,2}

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² School of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK

In this talk I will discuss two main advances in our understanding of transport and optics of massless Dirac fermions in encapsulated graphene. I will first report on results of combined theoretical and experimental work [1,2,3] showing unambiguous evidence for solid-state hydrodynamic DC transport. In particular, I will discuss how high-quality doped graphene sheets above liquid nitrogen temperatures exhibit *negative* non-local resistance near current injection points and whirlpools in the spatial current pattern [1,2,3]. Measurements of these non-local electrical signals allow to extract the value of the kinematic viscosity of the two-dimensional electron liquid in graphene, which is found to compare well with many-body theoretical predictions [4]. I will then present recent work [5] on viscous electron flow across graphene classical point contacts (see Fig. 1). Finally, I will describe near-field optical experiments [6] carried out in encapsulated graphene sheets where tunable quantum non-local effects have been discovered and theoretically analyzed.

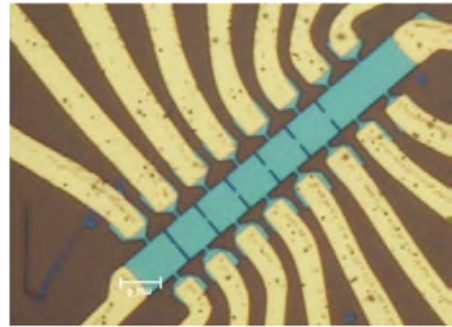


Fig. 1: A sequence of point contacts of varying width fabricated in encapsulated graphene (see Ref. 5)



Dr. Marco Polini graduated in Physics in 1999 from the University of Pisa (Italy) and received his Ph.D. in Physics in January 2003 from the Scuola Normale Superiore (Pisa, Italy). He is a Senior Scientist at the Istituto Italiano di Tecnologia in Genoa (Italy), where he leads the “Theory and technology of 2D materials” group. He is also Professor of Physics at the University of Manchester. Dr. Polini has co-authored more than 160 publications in peer-reviewed international journals including *Science*, *Nature Physics*, *Nature Materials*, *Nature Nanotechnology*, *Nature Photonics*, *Nature Communications*, and *Physical Review Letters* and the book “Many-body Physics in Condensed Matter Systems” (Edizioni della Normale, Pisa, 2006).

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Electronic, Thermal, and (Some) Unconventional Applications of 2D Materials

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Two-dimensional (2D) materials have applications in nanoelectronics and energy-conversion systems. These are also rich domains for fundamental discoveries as well as technological advances. This talk will present recent highlights from our research on graphene, h-BN, and transition metal dichalcogenides (TMDs).

We have studied graphene from basic transport measurements and simulations, such as velocity saturation [1], thermal conductivity [2], and self-heating effects in graphene field-effect transistors (GFETs) [3,4], to the recent demonstration of wafer-scale analog dot product nanofunctions for neural networks [5]. Taking advantage of its low *cross-plane* thermal conductance, we have found unexpected applications of graphene as an ultra-thin electrode to reduce power consumption in phase-change memory [6].

We have grown crystalline, monolayer TMDs by chemical vapor deposition (CVD) over cm² scales, including MoS₂ with low device variability [7,8], WSe₂, MoSe₂, and multilayer TMDs WTe₂ [9], ZrSe₂ and HfSe₂ which have native high-K dielectrics [10]. Improving the electrical contact resistance [11], we demonstrated 10-nm FETs using *monolayer* MoS₂, with the highest current density reported to date (>400 $\mu\text{A}/\mu\text{m}$), approaching ballistic transport limits [12].

In all high-field studies, device self-heating plays a key role, as predicted by our simulations [13] and confirmed by Raman thermometry (Fig. 1) [14]. Our Raman thermometry has also uncovered relatively low thermal boundary conductance (TBC $\sim 14 \text{ MW}/\text{m}^2/\text{K}$) between MoS₂ and SiO₂, which strongly limits heat dissipation in TMD-based electronics [14]. Additional studies are presently exploring unconventional applications including thermal switches. Thermal circuit elements could enable nanoscale control of heat in a manner similar to the control of current in electronic circuits.

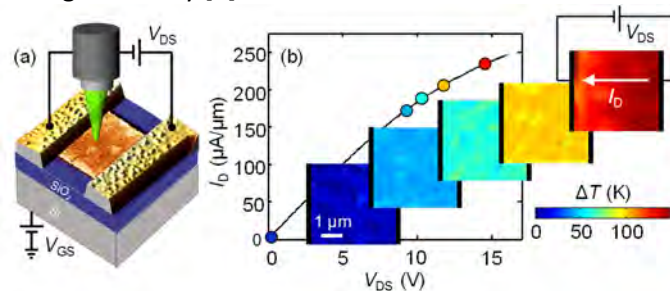


Fig. 1. (a) Schematic of Raman thermal measurement of monolayer MoS₂ FET during operation [12]. (b) Electrical *I-V* and Raman thermometry. Temperature maps correspond to the colored circles on the *I-V* curve. Measurements reveal low TBC $\sim 14 \text{ MW}/\text{m}^2/\text{K}$ between MoS₂ and SiO₂.



Eric Pop is an Associate Professor of Electrical Engineering (EE) and Materials Science & Engineering (by courtesy) at Stanford University. He was previously on the faculty of the University of Illinois Urbana-Champaign (2007-13) and also worked at Intel (2005-07). His research interests are at the intersection of nanoelectronics, nanomaterials, and energy. He received his PhD in EE from Stanford (2005) and three degrees from MIT (MEng and BS in EE, BS in Physics). His awards include the 2010 PECASE from the White House, the highest honor given by the US government to early-career scientists and engineers. He is also a recipient of Young Investigator Awards from the ONR, NSF CAREER, AFOSR, DARPA, of several teaching/advising awards, and best paper/poster awards with his students. He is an IEEE Senior member, he served as the General Chair of the Device Research Conference (DRC), and on program committees of the VLSI, IRPS, MRS, IEDM, and APS conferences. In a past life, he was a DJ at KZSU 90.1 FM from 2001-04. Additional information about the Pop Lab is available online at <http://poplab.stanford.edu>.

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Metalorganic Chemical Vapor Deposition of Transition Metal Dichalcogenides

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Future development of 2D devices based on transition metal dichalcogenide (TMD) monolayer and few-layer films requires the ability to synthesize large area, single crystal films and heterostructures. Our research is aimed at the development of an epitaxial growth technology for layered chalcogenides, similar to that which exists for III-V and II-VI compound semiconductors, based on gas source chemical vapor deposition (CVD) and metalorganic CVD (MOCVD) in cold-wall reactor geometries. This approach provides excellent control of the precursor partial pressure and reduced pre-deposition upstream of the substrate thereby enabling control over nucleation density, lateral growth rate and film composition for the growth of atomically-thin 2D films and heterostructures.

Our recent studies have focused on the epitaxial growth of WSe₂ and WS₂ monolayer films and vertical heterostructures on c-plane sapphire using metal hexacarbonyl and hydride chalcogen precursors. A multi-step growth method (Fig. 1) was developed which employs modulation of the metal precursor partial pressure to control the nucleation density, size and orientation and the lateral growth rate of domains on the substrate. Using this approach, coalesced monolayer and few-layer TMD films were obtained on sapphire substrates up to 2" in diameter at growth rates on the order of ~ 1 monolayer/hour. In-plane X-ray diffraction demonstrates that the films are epitaxially oriented with respect to the sapphire resulting from a merging of predominantly 0° and 60° oriented domains. This approach also provides a means to study and quantify surface diffusivities and lateral growth rates of domains as a function of growth conditions providing insight into the fundamental mechanisms of monolayer growth. Applications and challenges of this approach in the growth of 2D heterostructures will also be discussed.

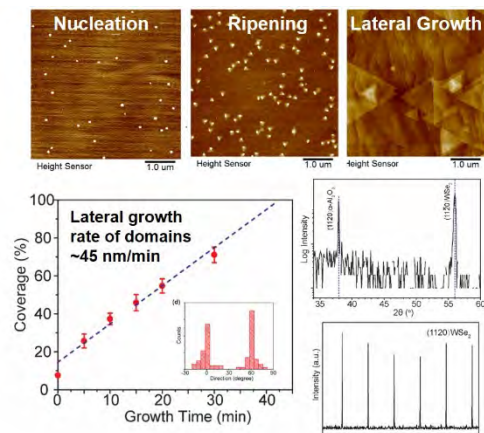


Figure 1. Multi-step process for epitaxial growth of WSe₂ on sapphire.



Joan M. Redwing received her Ph.D. in Chemical Engineering from the University of Wisconsin-Madison. After working as research engineer at Advanced Technology Materials Inc., she joined the faculty of the Department of Materials Science and Engineering at Penn State University in 1999. She holds an adjunct appointment in the Department of Electrical Engineering as serves as director of the 2D Crystal Consortium – Materials Innovation Platform. Her research focuses on understanding fundamental mechanisms of crystal growth and epitaxy of electronic materials, with a particular emphasis on thin film and nanomaterial synthesis by chemical vapor deposition. Dr. Redwing currently serves as vice president of the American Association for Crystal Growth and is an associate editor for the Journal of Crystal Growth. She is a fellow of the Materials Research Society, the American Physical Society and the American Association for the Advancement of Science and is a senior member of IEEE. She is an author or co-author on over 270 publications in refereed journals with over 11,000 citations and holds 8 U.S. patents.

Creating and Exploring Atomically-Thin Materials and Heterostructures

Joshua A. Robinson

Department of Materials Science & Engineering; The Center for 2D and Layered Materials; The Center for Atomically Thin Multifunctional Coatings; and The 2D Crystal Consortium
The Pennsylvania State University, University Park, PA 16802

The last decade has seen nearly exponential growth in the science and technology of two-dimensional materials. Beyond graphene, there is a huge variety of layered materials that range in properties from insulating to superconducting. Furthermore, heterogeneous stacking of 2D materials also allows for additional “dimensionality” for band structure engineering. In this talk, I will discuss recent breakthroughs in two-dimensional atomic layer synthesis and properties, including novel 2D heterostructures and novel 2D nitrides. Our recent works demonstrate that the properties of 2D materials, especially those grown via CVD, are extremely sensitive to the substrate choice. I will discuss substrate impact on 2D layer growth and properties, doping of 2D materials with magnetic elements, selective area synthesis of 2D materials, and 2D nitrides beyond hBN. Our work and the work of our collaborators has led to a better understanding of how substrate not only impacts 2D crystal quality, but also doping efficiency in 2D materials, and stabilization of nitrides at their quantum limit.

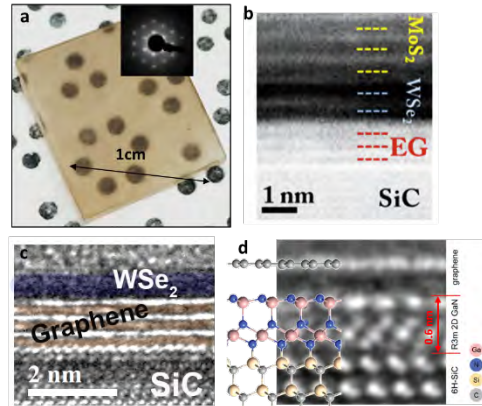


Fig.1: Examples of (a) wafer-scale WSe₂, (b,c) 2D heterostructures, and (d) 2D-Gallium Nitride.

Bio

Dr. Robinson obtained his B.S. degree in Physics with minors in Chemistry and Mathematics from Towson University in 2001. He received his doctorate degree from The Pennsylvania State University in Materials Science and Engineering in 2005. In 2012, he joined the Penn State Materials Science and Engineering Department as an Assistant Professor. In 2013, he co-founded the Center for Two-Dimensional and Layered Materials, and currently serves as Associate Director of the Center. In July 2015, he became Co-Director of the NSF I/UCRC Center for Atomically Thin Multifunctional Coatings (ATOMIC), and most recently, in 2016, he became the Director of User Programs for the NSF-funded 2D Crystal Consortium. He has authored or co-authored over 100 peer reviewed journal publications with a significant focus on low dimensional electronic materials. He has patents on chemical and neutron detection, and various pending patents related to 2D materials. Check out his research as <http://sites.psu.edu/robinsonresearch/>.



Van der Waals heterostructures for energy-efficient electronics
Prof. Tania Roy, University of Central Florida, United States

This talk will provide an update on electronic devices with van der Waals heterostructures. A vdW heterojunction-based all-two-dimensional transistor will be discussed. The all-2D transistor shows no surface roughness scattering, a property hitherto unforeseen in its three dimensional counterparts. A dual-gated MoS₂/WSe₂ vdW heterojunction diode can be tuned to operate in various diode operation regimes. The same device operates as a forward rectifying diode as well as a tunnel diode, merely by application of gate voltage. The first observation of gate controlled band-to-band tunneling in semiconducting 2D heterostructures was made here, enhancing the prospects of using vdW heterojunctions for low power electronic applications. A 2D/2D tunnel field effect transistor with WSe₂ and SnSe₂ will be discussed. Band-to-band tunneling induced negative differential resistance in WSe₂ homojunction devices will be shown. vdW heterojunctions with graphene/h-BN/graphene show negative differential resistance, which can be used in analog applications, such as in oscillators and amplifiers. A resistive memory built with graphene-insulator-graphene heterostructures, operating at sub-nW reset power will be demonstrated. An insight will be given into the reliability of vdW devices. By using the highly sensitive ‘conductance method’, the trap densities at a 2D/2D vdW interface has been extracted to be $<10^{11}$ states/cm²-eV. These results reinforce the case of vdW heterostructures unraveling a new paradigm in energy-efficient electronics.

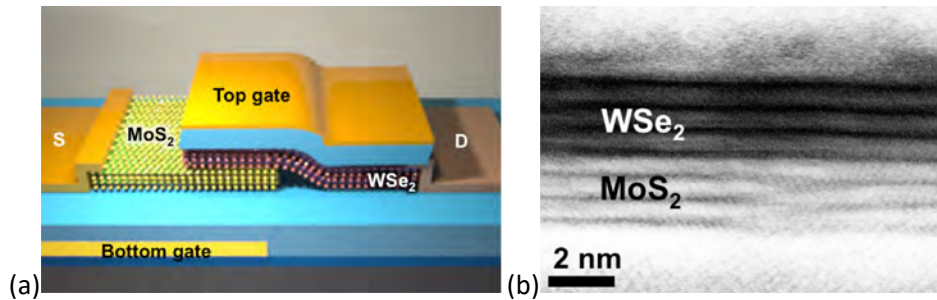


Figure 1. (a) Schematic of MoS₂/WSe₂ vdW heterojunction device. (b) Pristine, strain-free vdW interface as observed by HR-TEM.

Biography:

Dr Tania Roy joined University of Central Florida as Assistant Professor in 2016. She was a postdoctoral scholar at University of California, Berkeley from 2014-2016, working on 2D materials-based devices for low power electronics. She received B.E. (Hons.) degree in Electrical and Electronics Engineering from B.I.T.S. Pilani, India in 2006. She obtained her Ph.D degree in Electrical Engineering from Vanderbilt University, TN in December 2011, where she worked on the reliability of GaN/AlGaIn high electron mobility transistors for high power and high frequency electronics. Following that, she worked as a postdoctoral fellow at Georgia Institute of Technology on graphene-based devices for low power applications till 2013. Her research interests include using novel functional materials for energy-efficient electronics.

Transistors and steep transistors based on epitaxial 2D-materials, nanoribbons, and nanotubes

A. Seabaugh, C. Alessandri, M. Asghari, S. Fathipour, K. Gonzalez, L. Liu, P. Paletti, P. Pandey
University of Notre Dame, Notre Dame, IN

Susan Fullerton, University of Pittsburgh, Andy Kummel, University of California, San Diego
Chris Hinkle, KJ Cho, and Bob Wallace, University of Texas at Dallas, Maja Remskar, Jozef Stefan
Institute, Slovenia, and Joshua Robinson, Penn State

It is clearly feasible to achieve a steep subthreshold swing transistor with better energy efficiency than the MOSFET. The principles for lowering subthreshold swing are now well established, but technology for circuit development is only now emerging [1]. A sustained research and development effort is needed to meet the promise. Proofs in many material systems should now be reconsidered in the context of integration on a CMOS platform.

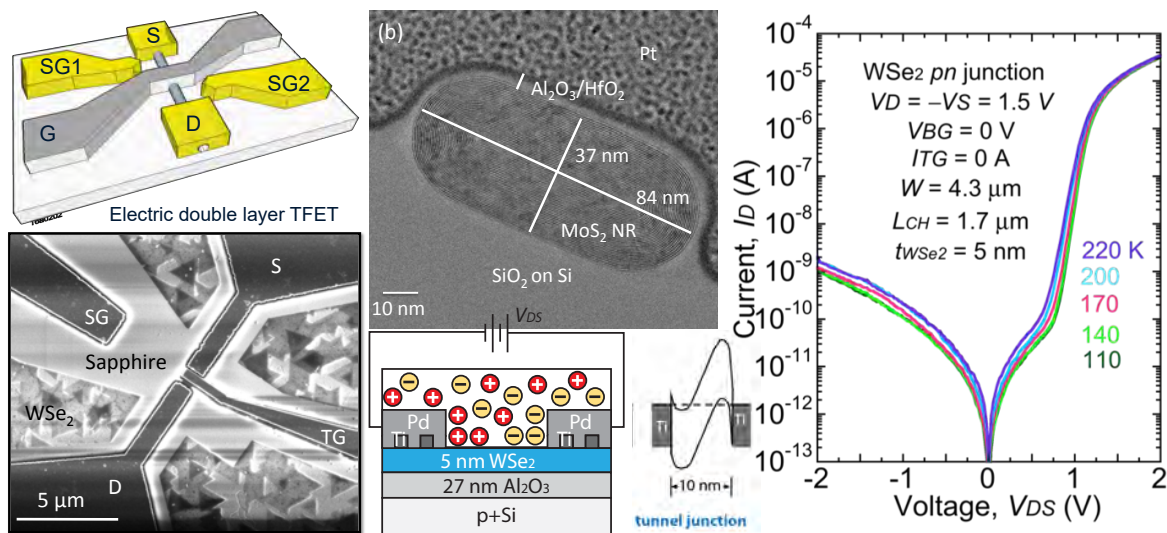


Fig. 1. Progress in tunnel field-effect transistors: doping, junction formation, and gate stacks.



Alan Seabaugh is the Frank Freimann Chair Professor of Electrical Engineering at the University of Notre Dame and Director of the STARnet Center for Low Energy Systems Technology. He received the Ph.D. in Electrical Engineering from the University of Virginia, Charlottesville, in 1985 and joined the University of Notre Dame in 1999, following positions at the National Bureau of Standards (1979-1986), Texas Instruments Incorporated (1986-1997), and Raytheon Systems Company (1997-1999). He has authored/ coauthored more than 300 papers and holds 24 U.S. patents. He served as editor for the IEEE Transactions on Electron Devices (2010-2015) and is an IEEE Fellow. He received the International Symposium on Compound Semiconductor Quantum Devices Award in 2011 for seminal contributions and leadership in semiconductor devices and circuits based on quantum-mechanical tunneling.

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Controlling Filament Dynamics in Resistive Switching Devices with 2D Interlayers

Nikhil Shukla

Department of Electrical and Computer Engineering, University of Virginia

Resistive switching devices are being actively explored for a wide range of applications ranging from non-volatile memory to neuromorphic computing. While such devices have shown promising switching properties such as ON/OFF ratio and low power operation, the large variability (cycle to cycle, and device-to-device) continues to pose a challenge. This behavior arises from the inherent stochasticity in filamentary dynamics

(example, multiple filament formation, filament diameter); thus, overcoming the variability bottleneck entails a solution that enables enhanced control of the filament formation and rupture properties. In this work, we investigate 2D materials such as graphene as interlayers to regulate the filamentary dynamics in Ag/HfO₂ based Conducting-Bridge RAM devices. The effects of the 2D interlayer on the resistive switching properties, particularly the variation and reliability, will be discussed.

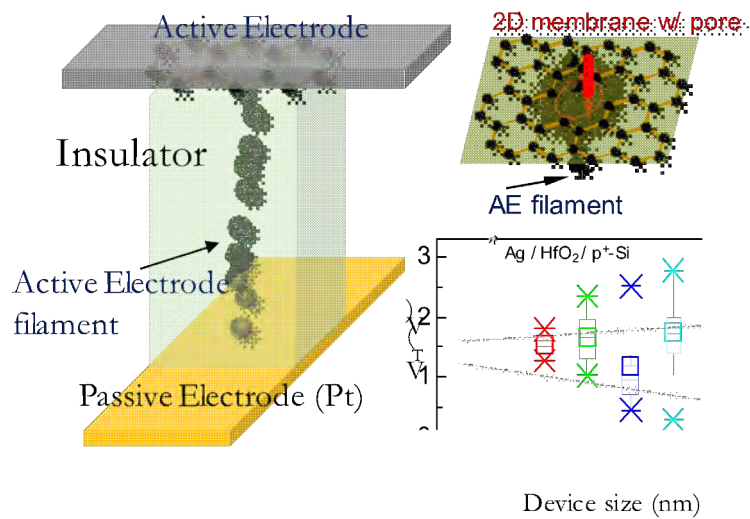


Fig. 1 Schematic of Ag/HfO₂-based CB-RAM device with graphene interlayer; scaling of V_T variation with device size.



Nikhil Shukla will be starting as an Assistant Professor at University of Virginia in January 2018 with a joint appointment in the ECE and the Materials Science and Engineering department. He completed his BS in Electronics and Telecommunications from the University of Mumbai, India, in 2010, and a PhD in Electrical Engineering from the University of Notre Dame in 2017. His research interests lie in emerging devices and circuits as well as developing new approaches for energy efficient computing and storage. He received the best publication award from the STARnet Center for Low Energy Systems Technology (LEAST) for three consecutive years 2015, 2016, and 2017, as well as the best paper award 2017 from IEEE TMSCS. He is the recipient of the J.N. TATA and the JRD Tata Scholarships, India.

Van der Waals Layered Materials: Building the Knowledge-Base, Synthesis and Devices for the New Frontier in Nanophotonics

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We discuss cataloguing, categorizing, synthesizing, characterizing, and validate a broad range of van der Waals layered materials as candidates for optical and photonic applications towards accelerating the time frame from material conception to application-near deployment. We show how utilizing advanced computation methods enable screening hundreds of thousands of crystalline systems for the potential to form 2-dimensional (2D) materials. Our results include the establishment of a database of over 1000 layered materials by data mining the Materials Project. Here we discovered that there are approximately 100 materials that have either been mined or synthesized that are layered, but consist of more than one type of layer. These are essentially bulk 3D analogs to the vertical heterostructures that many researchers are attempting to create mechanically in the lab. We studied phases of 2D materials to in-situ control their properties, and performed computational screening of the ability of adsorbates to stabilize phases was conducted. Experimentally, we validated the growth of the 1T phase of MoTe₂ in the presence of CO₂ in the process gas highlighting the viability of the computationally predicted approach. Furthermore, we find that varying the growth method allows the formation of hybrid films of mixed phases that exhibit susceptibility to gating and significantly increased conductivity. Towards delivering direct on-chip synthesis capabilities, we developed a new method to integrate CVD-grown TMDs with plasmonic cavities, and show that using these cavity-2D material heterostructures allow for E-field field enhancement in the center of a bow-tie or dimer plasmon cavity, yet the field enhancement vanishes when the TMD is placed some in a quenching-save distance away from the plasmon cavity. Here we find that the PL emission enhancement of plasmon cavities depends critically on the relative position of the TMD WRT the field enhancement of the cavity. Moreover, we demonstrated 2D material interactions with surface acoustic waves on-chip. We developed a novel 2D material transfer setup that improves both accurately and cross-contamination compared to all other transfer setups, allowing for on-demand printing of 2D Materials. Lastly, we show how the strong exciton binding energy of TMDs can be harnessed to design attojoule per bit efficient electro-optic modulators.



Volker J. Sorger is an associate professor in the Department of Electrical and Computer Engineering, and the director of the Orthogonal Physics Enabled Nanophotonics (OPEN) lab at the George Washington University. He received his PhD from the University of California Berkeley. His research areas include optoelectronic devices, plasmonics and nanophotonics, including novel materials, and optical analogue information processing and neuromorphic computing. Amongst his breakthroughs are the first demonstration of a semiconductor plasmon laser, diffraction-limited waveguides, and sub 1-Volt plasmonic electro-optic modulator, optical FFT on-chip, and symmetry-detection via neuromorphic computing. Dr.

Sorger received multiple awards among are the Early Career Award and Dean's Outstanding Young Research Award at GW, the AFOSR Young Investigator Award, Hegarty Innovation Prize, and the National Academy of Sciences award of the year. Dr. Sorger is the editor-in-chief of Nanophotonics, the executive chair overseeing all Technical Groups at OSA, and serves at the board-of-meetings at OSA and SPIE and the scholarship committee. He is a senior member of IEEE, OSA & SPIE.

Ballistic transport in CVD graphene

C. Stampfer, L. Banszerus, M. Schmitz, and B. Beschoten

JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Germany

In order to advance from basic graphene research towards scalable industrial applications, large area high quality graphene is needed. One promising approach to achieve this is chemical vapor deposition (CVD) of graphene on (reusable) copper. However, so far the charge carrier mobility of CVD grown graphene has been significantly lower than what has been observed in devices fabricated from exfoliated graphene. I will show that the electronic quality of CVD graphene depends critically on the transfer method and we present a novel dry transfer technique for CVD-grown graphene crystals that yields devices encapsulated in hexagonal boron nitride (hBN) with carrier mobilities up to $350,000 \text{ cm}^2/\text{Vs}$ [1]. In addition to the diffusive transport in such samples, we demonstrate an elastic mean free path exceeding one micrometer at temperatures of up to 200 K using Hall cross devices. By investigating large samples (see e.g. Fig. 1) we furthermore conclude that the mean free path can exceed 25 micrometer at 2 K [2]. Thus, in summary we show that by choosing the right substrates [3] the electronic properties of CVD grown synthetic graphene matches those of ultrahigh-mobility exfoliated natural graphene.

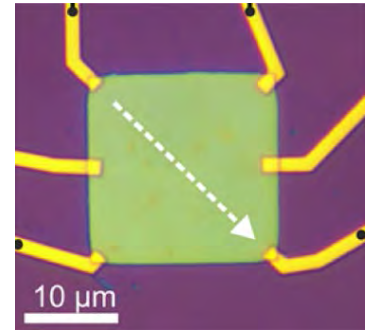


Fig. 1. Optical image of a CVD graphene/hBN heterostructure exhibiting ballistic transport.

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[2] L. Banszerus, M. Schmitz, S. Engels, M. Goldsche, K. Watanabe, T. Taniguchi, B. Beschoten and C. Stampfer, *Nano Letters* **16**, 1387 (2016).

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Christoph Stampfer is Professor of Experimental Solid State Physics at the RWTH Aachen University and researcher at the Forschungszentrum Jülich. He is primary interests include graphene and 2D materials research, mesoscopic transport, and micro electromechanical systems. He holds a Dipl.-Ing. Degree in Technical Physics from the TU Vienna and a Ph.D. in Mechanical Engineering from the ETH Zurich. He was a staff member at the Institute for Micro and Nano Systems of the ETH Zurich from 2003 to 2007 and staff member of the Institute for Solid State Physics (ETH Zurich)

from 2007 to 2009. From 2009 till 2013 he was JARA-FIT Junior Professor at the RWTH Aachen and the Forschungszentrum Jülich. He has been awarded with an ERC Starting Grant to work on "Graphene Quantum Electromechanical Systems" in 2011 and is member of the Young Scientist community of the World Economic Forum since 2014.

Direct Observation of the Josephson Inductance of a Ballistic Graphene Josephson Junction using a Superconducting Cavity

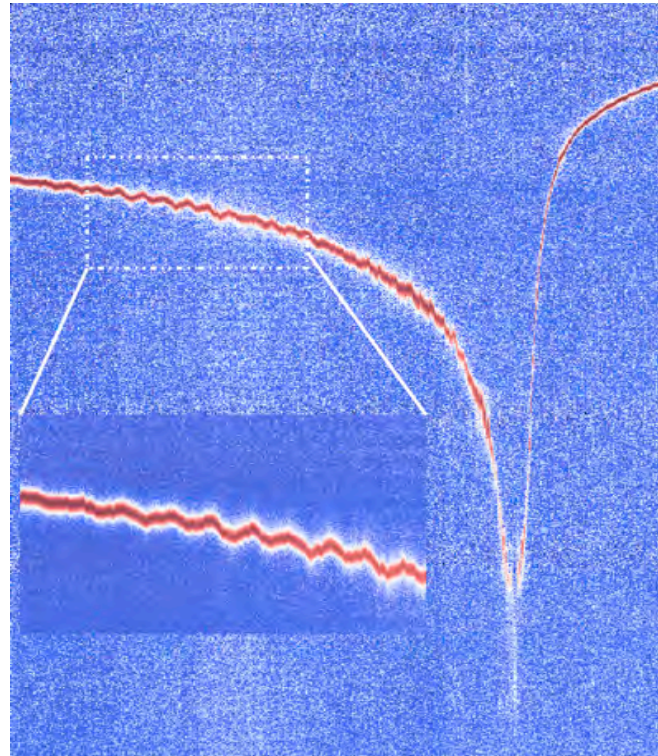
Felix Schmidt, Mark Jenkins, Gary Steele
Kavli Institute of Nanotechnology, 2628 CJ Delft, The Netherlands

K. Watanabe, T. Taniguchi
National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

In this talk, I will present our recent work incorporating ballistic graphene Josephson junctions into superconducting quantum microwave circuits. Graphene junctions offer the potential for quantum circuits, such as cavities and qubits, whose frequency would be tunable by electric fields. Conversely, such circuits also enable the direct observation of the Josephson inductance of the graphene junction, a parameter not accessible in conventional DC transport measurements.

In our device, a Josephson junction made from high-mobility single-layer graphene encapsulated in boron nitride is embedded in a superconducting microwave cavity. The cavity has a unique design that also allows simultaneous measurement of the current-voltage (IV) characteristics of the junction, and to apply gate voltages without spoiling the quality-factor of the cavity.

Sweeping the gate voltage, we observe tuning of the cavity in response to the changing Josephson inductance of the junction, directly observing the Dirac peak of graphene layer and ballistic quantum interference oscillations in the cavity frequency. From the cavity frequency and an RF model of our device, we can extract the Josephson inductance quantitatively, revealing detailed information of the current-phase relation at energy scales down to the level of a single photon. Finally, we explore dissipation in the device, use our RF device model to extract the density dependence of the subgap resistance, and evaluate the potential of ballistic graphene junctions for applications in quantum technologies.



Dr. Gary Steele, born in Toronto, Canada, obtained his Ph. D. from MIT in 2006, working with Prof. Raymond Ashoori on scanning capacitance imaging of the quantum Hall liquid. After his Ph. D., Gary moved to the Kavli Institute of Nanoscience in Delft, where he worked with Prof. Leo Kouwenhoven on ultraclean carbon nanotube quantum dots. In 2010, he obtained a position as a tenure-track assistant professor at the Kavli Institute in Delft working on nanomechanics, with a focus in recent years on mechanical resonators and quantum microwave circuits. Since 2015, Gary is a tenured Associate Professor in Delft.



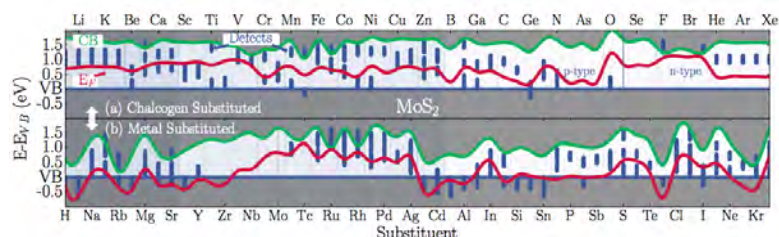
Ab initio studies of TMDs: new doping avenues and TMD/metal interfaces

Alejandro Strachan

School of Materials Engineering and Birck Nanotechnology Center
Purdue University, West Lafayette, Indiana, 47906 USA

The potential of transition metal dichalcogenides (TMDs) for a range of applications is well established but several challenges must be overcome before their full potential is realized. In this presentation, I will discuss density functional theory calculations to explore doping of TMDs and their

interfaces with metals. A high-throughput study of doping of molybdenum and tungsten dichalcogenides with a large fraction of the periodic table provides insightful trends across the periodic table and points out promising dopants to be pursued experimentally. Beyond previously studied cases, our predictions suggest promising substitutional dopants that result in p-type transport and reveal interesting physics behind the substitution of the metal site. Substitutional doping of the metal site with early transition metals (TMs) results in p-type doping and n-type can be achieved with mid TMs. Quite interestingly, the simulations indicate the possibility of interstitial doping of TMDs; the energetics reveal that a significant number of dopants, specially for ditellurides, favor the interstitial sites over adsorbed ones. This suggests that interstitial impurities in TMDs are more common than thought to date and we propose a series of potential interstitial dopants. Interfaces between TMDs and metals are also key to their integration into devices and I will discuss the mechanical and electronic properties of the interface between several single-layer TMDs and Cu(111). The electronic structure of the interfaces indicates partial covalent bonding and a complex redistribution of electronic density. The resulting net electric dipoles significantly alter the electron work function of the Cu surface. Capping Cu(111) surfaces with Group IV and V TMDs leads to an increase in the work function of up to 1 eV while Group VI TMDs can decrease the work function by up to 1 eV.



Alejandro Strachan is a Professor of Materials Engineering at Purdue University and the Deputy Director of the Purdue's Center for Predictive Materials and Devices (c-PRIMED) and of NSF's Network for Computational Nanotechnology. Before joining Purdue, he was a Staff Member in the Theoretical Division of Los Alamos National Laboratory and worked as a Postdoctoral Scholar and Scientist at Caltech. He received a Ph.D. in Physics from the University of Buenos Aires, Argentina, in 1999. Among other recognitions, Prof. Strachan was named a Purdue University Faculty Scholar (2012-2017), received the Early Career Faculty Fellow Award from TMS in 2009 and the Schuhmann Best Undergraduate Teacher Award from the School of Materials Engineering, Purdue University in 2007. Prof. Strachan's research focuses on the development of predictive atomistic and molecular simulation methodologies to describe materials from first principles, their application to problems of technological importance and quantification of associated uncertainties. Application areas of interest include: coupled electronic, chemical and thermo-mechanical processes in devices of interest for nanoelectronics and energy as well as polymers and their composites, molecular solids and active materials, including shape memory and high-energy density materials.



Second Harmonic Generation of Transition Metal Dichalcogenides Alloys and BNC Alloys

Humberto Terrones
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The advances in growth methods is allowing the possibility of synthesizing alloys of 2-D materials: To shed light on their nonlinear optical properties, first principles calculations have been used to calculate the second harmonic generation (SHG) of alloys of transition metal dichalcogenides (TMDS) and BNC layered systems. The results obtained indicate that chalcogen alloys of the type MoSSe or WSSe are more suitable for SHG applications than alloys of the type MoWS₄ or MoWSe₄ (see Figure 1).

Additionally, zigzag nanotubes made from the above mentioned alloys have been considered and it is found that as their diameter gets smaller the intensity of the SHG is higher. Surprisingly, the intensity of the SHG in TMDs Haeckelites of the type NbSSe and Nb_{0.5}Ta_{0.5}S₂ exhibit the highest intensity for the SHG. The study was extended to BNC alloy systems of the type BNC₂, B_xN_xC_y Haeckelites and porous BN (BN

Schwarzites). It is found that BNC₂ possesses much higher SHG than h-BN, making this a suitable material

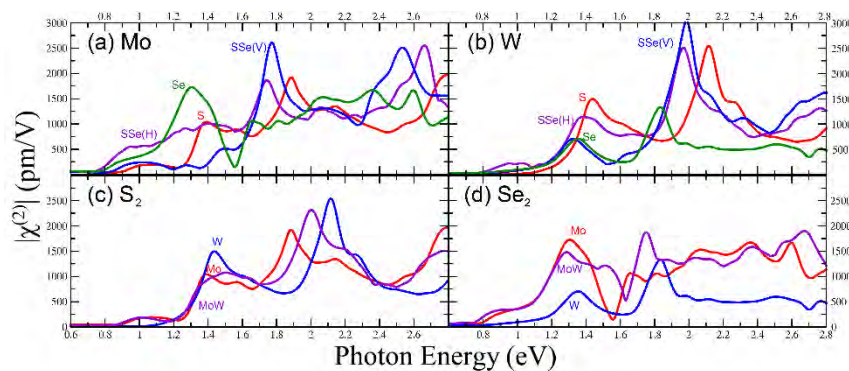


Fig.1 Magnitude of the second order susceptibility $\chi^{(2)}$ for different TMDs alloys.

for non-linear optical properties. BN Schwarzites can be compared with the highest SHG 3-D materials found so far.

Humberto Terrones is Rayleigh Endowed Chair Professor in Physics at Rensselaer Polytechnic Institute. He obtained his BSc from Iberoamericana University, Mexico, his PhD from University of London (Birkbeck) and carried out a postdoctoral stay in Cambridge (UK). He has been visiting professor in Brazil, US, Japan and Belgium. He has around 280 papers in refereed journals with an h-index of 83 according to Google Scholar. He is a member of the Mexican Academy of Sciences, The World Academy of Sciences for the Advancement of Science in the Developing World (TWAS) and Fellow of the American Physical Society.



2D Topological Insulator Electronics

William Vandenberghe¹

¹Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, TX

Two-dimensional (2D) topological insulators (TIs) are 2D semiconductors that distinguish themselves from 'conventional' 2D semiconductors (like monolayer hBN or MoS₂) by the presence of electronic states on their edges. These TI edge states traverse the bandgap and exhibit spin-momentum locking. The spin-momentum locking prohibits intra-edge scattering giving rise to extraordinarily



Fig. 1 Schematic operating principle a topological insulator-based FET in the on-state (left) and in the off-state (right).

efficient electronic transport. Electronic transport will proceed efficiently along the TI edge states as long as the Fermi level is positioned in the bandgap of the 2D TI. If the Fermi level in the 2D TI is close to or lies in the bulk conduction or valence band, scattering is no longer prohibited and can dramatically reduce the conductivity of the 2D TI. Gating a 2D TI enables the modulation of the Fermi level and subsequently the current, realizing a 2D TI field-effect transistor (FET) whose operating principle is illustrated in Fig. 1. Based on simulated input- and output characteristics, we have estimated the intrinsic switching energy and delay as $E_{\text{int}}=0.42\text{aJ}$ and $t_{\text{int}}=0.22\text{ps}$. We have also estimated the switching energy and delay for a TIFET arithmetic logic unit (ALU). Comparing the delay and energy, the TIFET-based performs better in benchmarking compared to all other alternative proposed low-power devices. Overall, the high electron velocity of the edge states results in a low density-of-states and only a small amount of charge is required to switch a TIFET resulting in an energy-efficient switch. Combining this with the robustness against imperfections (e.g. defects/edge roughness), the TIFET a promising candidate for future low-power high-performance device applications.



Dr. William Vandenberghe is an assistant professor in the Materials Science Department (MSE) at the University of Texas at Dallas (UTD) since 2016. He received the M.Sc. degree (magna cum laude) and the Ph.D. degree in Electrical Engineering from the Katholieke Universiteit Leuven (KU Leuven), Belgium in 2007 and 2012 respectively. Work for his Ph.D. was supported by a fellowship and conducted at imec, an international renowned research institute that performs research in different fields of nanoelectronics headquartered in Leuven, Belgium. From 2012-2016, he was a research associate/scientist in the MSE department at UTD. He has an h-index of 19, a total citation count of 1577, and has authored 60 peer-reviewed documents

to date. He is an author of a 474-page Springer Graduate Texts in Physics "Advanced Physics of Electron Transport in Semiconductors and Nanostructures" published in 2016. He is an associate editor for the Journal of Computational Electronics. He has published in high-impact journals such as ACS Nano and authored a first author publication in Nature Communications in 2017. In 2014, he was the recipient of the KU Leuven research council award, annually awarded to a single Ph.D. thesis in the field of applied sciences. In 2017, he received a research award from the National Science Foundation (NSF) and the Young Investigator Award from the Defense Threat Reduction Agency (DTRA). His research interest goes towards the theoretical study of novel materials and devices for electronic applications.

Spintronics in Van der Waals heterostructures

Bart van Wees

Zernike Institute for Advanced Materials

University of Groningen

Graphene is an ideal material to transport electronic spins, because of its very low spin-orbit interaction, allowing in theory spin transport 1mm distance at room temperature. However, this also implies that spins in graphene are difficult to manipulate and control. In this talk I will first introduce the basic notions of spintronics in graphene. Then I will show that by stacking the graphene on or in between Van der Waals materials, we can optimize the spin transport in graphene and also induce new functionalities, such as anisotropic spin orbit interaction and ferromagnetism. I will discuss the following:

- 1) By encapsulation with crystalline hexagonal boron nitride we showed that, by using carrier drift, spins can be transported over distances of 90 micrometer or more. [1]
- 2) We have found that using a hBN bilayer as tunnel barrier for spin injection/detection we can dramatically increase the efficiencies as well as the spin signals. [2]
- 3) By exfoliation graphene on a ferromagnetic insulator (yttrium iron garnet (YIG)) we have been able to induce an proximity exchange interaction, thus making the graphene effectively ferromagnetic. We have measured the effect of the exchange field on the spin precession. [3]
- 4) By studying spin transport in a single layer graphene/single layer transition metal dichalcogenide sandwich we can proximity induce an anisotropic spin orbit interaction in graphene, resulting in large difference of the relaxation of spins with in-plane and out-of-plane direction. [4]

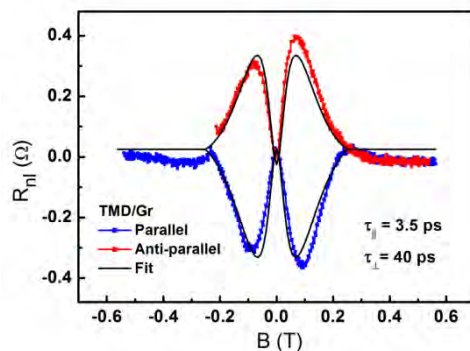


Fig. 1. Hanle spin precession, due to an in-plane magnetic field, showing the increase of the spin signal due to the precession of in-plane spins into out-of-plane spins with larger spin lifetimes (from ref. [4])

1] J. Ingla-Aynés et al. "Eighty-eight percent directional guiding of spin currents with 90 micrometer relaxation length in bilayer graphene using carrier drift", [Nano Letters 16, 4825 \(2016\)](#)

2] J.C. Leutenantsmeyer, et al., "Proximity induced room-temperature ferromagnetism in graphene probed with spin currents", [2D Mater. 4, 014001 \(2017\)](#)

3] M. Gurram, et al., "Bias induced up to 100% spin-injection and detection polarizations in ferromagnet/bilayer-hBN/graphene/hBN heterostructure", [Nature Comms. 8, 248 \(2016\)](#).

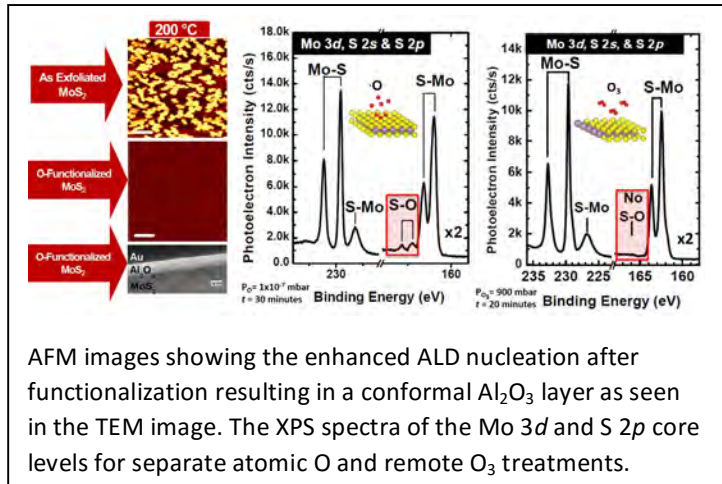
4] T. S. Ghiasi, et al., "Proximity-Induced Spin Lifetime Anisotropy in Transition Metal Dichalcogenide/Graphene Heterostructures", [arXiv:1708.04067](#), subm. to Nano Lett.

2D Materials Integration: What have we learned?

Robert M. Wallace

University of Texas at Dallas, Richardson, Texas, USA

The size reduction and economics of integrated circuits, captured since the 1960's in the form of Moore's Law, continues to be challenged. Challenges include addressing aspects associated with truly atomic dimensions, while the cost of manufacturing is increasing such that only 3 or 4 companies can afford leading edge capabilities. To address the physical limitations, 2D materials such as graphene, phosphorene, h-BN, and transition metal dichalcogenides have captured the imagination of the electronics community for advanced applications in nanoelectronics and optoelectronics. The ideal materials properties have much appeal, but the reality of defects, impurities, and materials integration constraints will surely compromise the intrinsic performance of such device technologies. This talk will present a sample of our recent work examining defects, impurities, functionalization, as well as the process integration challenges and potential solutions.¹



AFM images showing the enhanced ALD nucleation after functionalization resulting in a conformal Al_2O_3 layer as seen in the TEM image. The XPS spectra of the Mo 3d and S 2p core levels for separate atomic O and remote O_3 treatments.

This work was supported in part by the Center for Low Energy Systems Technology (LEAST), one of the six SRC STARnet Centers, sponsored by MARCO and DARPA, the Southwest Academy on Nanoelectronics (SWAN) Center, a SRC center sponsored by the Nanoelectronics Research Initiative and NIST, and the US/Ireland R&D Partnership (UNITE) under the NSF under award ECCS-1407765.



Dr. Wallace is a Professor of Materials Science and Engineering and holds the Erik Jonsson Distinguished Chair in the Jonsson School of Engineering and Computer Science at the University of Texas at Dallas. He received his Ph.D. (1988) in Physics at the University of Pittsburgh. In 1990, he joined Texas Instruments Central Research Laboratories as a Member of Technical Staff (MTS) in the Materials Characterization Branch of the Materials Science Laboratory, and was elected as a Senior MTS in 1996. Dr. Wallace was then appointed in 1997 to manage the Advanced Technology branch in TI's R&D which focused on advanced device concepts and the associated material integration issues. In 2003, he joined the faculty at UTD. Dr. Wallace also has appointments in the Departments of Electrical Engineering, Mechanical Engineering, and Physics. Dr. Wallace is also an inventor on 45 US and 27 international patents/applications, and was named Fellow of the AVS in 2007 and an IEEE Fellow in 2009 for his contributions to the field of high-k dielectrics in integrated circuits. He has authored or co-authored over 360 publications in peer reviewed journals and proceedings with over 19000 (28000) citations according to Scopus (Google Scholar).

¹ S. J. McDonnell and R.M. Wallace, "Critical Review: Atomically-Thin Layered Films for Device Applications based upon 2D TMDC Materials", *Thin Solid Films*, 616, 482-501 (2016).

Black Phosphorus Optoelectronics and Electronics

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Black phosphorus recently emerged as a promising new 2D material due to its widely tunable and

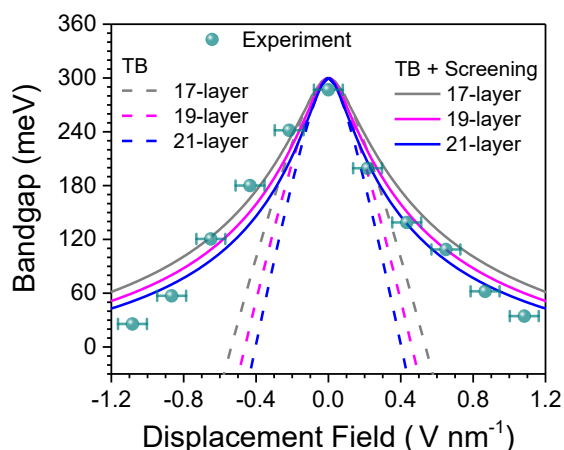


Figure 1. Efficient tuning of thin-film black phosphorus bandgap. Adapted from Nat. Commun. 8, 14474 (2017).

direct bandgap by layer number, high carrier mobility and remarkable in-plane anisotropic electrical, optical and phonon properties. It serendipitously bridges the zero-gap graphene and the relatively large bandgap transition metal dichalcogenides such as molybdenum disulphide (MoS₂). In this talk, I will first cover the basic properties of few-layer and thin-film black phosphorus, followed by a discussion on recent progress on black phosphorus synthesis. Finally, I will present results on bandgap tuning in few-layer and thin-film black phosphorus. These recent developments further reveal the promising future of black phosphorus in advanced electronics and integrated nanophotonics.



Fengnian Xia received the B.E. degree with highest honor in electronics engineering from Tsinghua University, Beijing, China and Ph.D. degrees in electrical engineering from Princeton University, Princeton, NJ, USA. He joined IBM Thomas J. Watson research center in Yorktown Heights, NY, USA as a postdoc in 2005, and was a Research Staff Member before he started at Yale University in September 2013. Currently he is the Barton L. Weller associate professor in engineering and science at Department of Electrical Engineering. He currently explores the light-matter interaction and quantum transport in low-dimensional materials and

also identifies their potential applications in computing, flexible electronics, imaging, optical communications, and energy harvesting.

Monolayer Magnets

Xiaodong Xu

Department of Physics, Department of Materials Science and Engineering
University of Washington, Seattle WA

Since the discovery of graphene, the family of two-dimensional (2D) materials has grown to encompass a broad range of electronic properties. However, until recently 2D crystals with intrinsic magnetism were still lacking. Such crystals would enable new ways to study 2D magnetism by harnessing the unique features of atomically-thin materials, such as electrical control for magnetoelectronics and van der Waals engineering for novel interface phenomena. In this talk, I will describe our recent magneto-optical spectroscopy experiments on van der Waals magnets, chromium(III) iodide CrI_3 . I will first demonstrate the existence of isolated monolayer semiconductor with intrinsic Ising ferromagnetism. I will then show the layer number-dependent magnetic phases. The magnetic ground state evolves from being ferromagnetic in a monolayer, to antiferromagnetic in a bilayer, and back to ferromagnetic in a trilayer and thin bulk. Lastly, I will discuss the emerging spin phenomena in monolayer $\text{WSe}_2/\text{CrI}_3$ ferromagnetic semiconductor heterostructures, including ferromagnetic control of valley pseudospin in WSe_2 via large magnetic exchange field, and optical analog of giant magnetoresistance effect.

Wafer-Scale 2D MOSFET Fabrication on CVD MoS₂ and CMOS Substrate

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We successfully developed an alternative to the current practice of mechanical exfoliation and electron-beam lithography in fabricating 2D MOSFETs. The alternative uses photolithography on large-area monolayer MoS₂ grown by chemical vapor deposition and transferred onto a silicon substrate fabricated by the CMOS back-end-of-line (BEOL) process. The BEOL process allows buried aluminum gates as short as 0.2 μm and high-quality gate insulator to be fabricated before MoS₂ transfer (Fig. 1). After further CMOS-compatible photolithography processes, approximately 200,000 RF-probable MoS₂ MOSFETs could be fabricated on a 200-mm-diameter high-

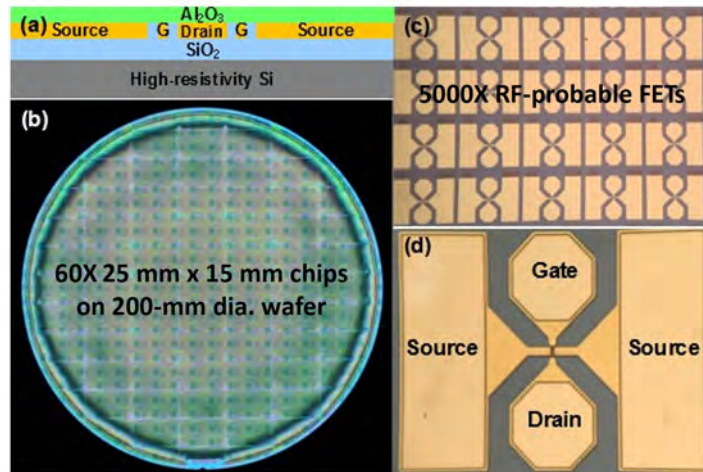


Fig. 1. (a) Cross-section schematic of a buried-gate MOSFET and micrographs of (b) a 200-mm dia. wafer, (c) a 25-mm by 15-mm chip, and (d) a MOSFET.

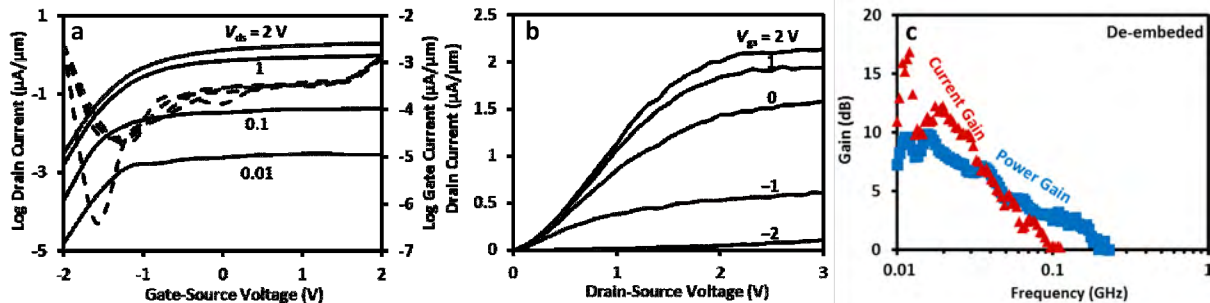


Fig. 2. (a) Transfer characteristics, (b) drain characteristics, and (c) current gain and power gain of a typical MoS₂ MOSFET.

resistivity Si wafer. The resulted MOSFETs had $> 10^3$ on/off ratio, approximately 10 cm²/Vs electron mobility, and 100 MHz cutoff frequencies (Fig. 2).



Kuanchen Xiong received his BE degree in Electronic Science and Technology from Southeast University in 2015. He then joined the research group of Professor James C. M. Hwang at Lehigh University, Department of Electrical and Computer Engineering. His current research interest focuses on the 2D semiconducting materials, nano-electronic devices, and CMOS-compatible process based on 2D materials.

High Performance Transistor Technology Enabled by 2D and 1D van der Waals Materials

Peide D. Ye

School of Electrical and Computer Engineering, Purdue University, USA

2D materials research and their related physics and chemistry studies are the foundation for 2D nanoelectronics and photonics development. In this talk, we will review the state-of-the-art 2D semiconductor materials research and development in the recent years and highlight a couple of new breakthroughs at our research group such as (1) integration of CMOS compatible ferroelectric HfZrO_2 gate stack on 2D materials to realize steep slope negative capacitance field-effect transistors (2) realization of black phosphorus 2D transistors with record drain currents beyond $1\text{A}/\text{mm}$ (3) exploration of a new class of 1D van der Waals materials – Te and Se – which has narrow bandgap, high carrier mobility and air stability. The research is in close collaborations with 2DARE Phosphorene Team and also Profs. Wenzhuo Wu, Ashraf Alam, Ali Shakouri's groups at Purdue University.



Dr. Peide Ye is Richard J. and Mary Jo Schwartz Professor of Electrical and Computer Engineering at Purdue University in USA. He received Ph.D. from Max-Planck-Institute of Solid State Research, Stuttgart, Germany, in 1996. Before joining Purdue faculty in 2005, he worked for NTT Basic Research Laboratory, NHMFL/Princeton University, and Bell Labs/Lucent Technologies/Agere Systems. His current research work is focused on atomic layer deposition technology and its device integration on novel channel materials including III-V, Ge, graphene, 2D materials and complex oxides. He authored and co-authored more than 200 peer reviewed articles and 350 conference presentations including many invited, keynote and plenary talks. He also served as chairmen and program committee members on top international conferences and symposia. He is a Fellow of IEEE and APS (American Physical Society).

Nanoscale Electronic and Photonic Devices Based on Two-dimensional Materials

Wenjuan Zhu

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Two-dimensional (2D) materials are layered crystals with strong in-plane covalent bonds and weak interlayer van der Waals bonds. These materials have many unique chemical, mechanical, optical and electrical properties, which not only provide a platform to investigate fundamental physical phenomena but also may provide solutions to some of today's most pressing technological challenges. In this meeting, I will present our work on understanding the electrical properties of graphene, transition metal dichalcogenides, black phosphorus, group IV chalcogenides, and their heterostructures.¹⁻³ I will also present our work on the nano-scale electronic devices (logic devices and radio frequency devices) and photonic devices (plasmonic devices and photo-detectors) based on these 2D materials.⁴⁻⁶

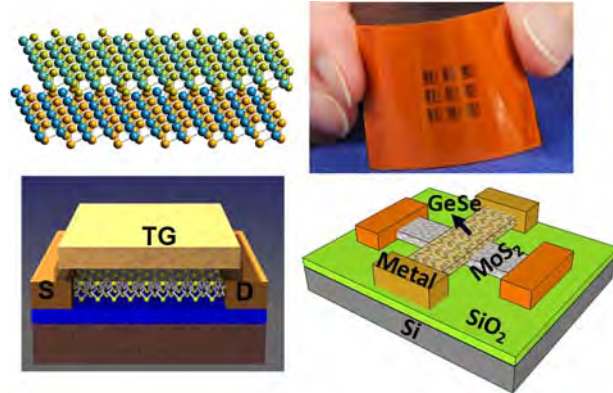


Figure 1. Illustration of 2D crystals and nanoscale devices based on 2D materials.



Wenjuan Zhu is an assistant professor in Department of Electrical and Computer Engineering at University of Illinois at Urbana-Champaign. Wenjuan Zhu received her Ph.D. degree in the Department of Electrical Engineering at Yale University in 2003. After graduation, she joined IBM Semiconductor Research and Development Center. She made key contributions to the 65nm and 32nm CMOS technology nodes. In 2008, she joined the IBM T. J. Watson Research Center and worked on 2D materials including graphene and layered transition metal dichalcogenides. In 2014, she joined the faculty at the University of Illinois and established a research group focusing on two-dimensional (2D) materials and nanoscale devices. Her research in the past has resulted in more than 80 publications in journals/conferences and 24 patents issued/pending. Prof. Zhu received National Science Foundation CAREER award in 2017, IBM Research's Pat

Goldberg Memorial Best Paper Award in 2013, Outstanding Technical Achievement Award in IBM in 2008, more than ten Invention Achievement Award in IBM, Henry Prentiss Becton Graduate Prize for exceptional achievement in research in Engineering and Applied Science at Yale University in 2003.

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