Workshop on Simulation and Modeling of Emerging Electronics (SMEE) 2018

October 15 – 16, 2018

Room KK LG101, K.K. Leung Building, HKU

Organizing Committee

Prof. Jian Wang (HKU)
Prof. Hong Guo (HKU & McGill U.)
Prof. Fuchun Zhang (HKU & UCAS)
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Workshop on Simulation and Modeling of Emerging Electronics (SMEE) 2018 Program

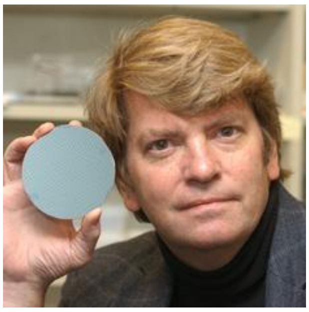
Eight year of the Area of Excellence (AoE) on Theory, Modeling, and Simulation of Emerging Electronics

Monday, October 15, 2018		
08:20 - 09:00 Registration		
Chairperson: Prof. Hong Guo, HKU&McGill		
08:40 - 09:00	Welcome Address and Photo taking **Jian Wang,** The University of Hong Kong	
09:00 - 09:45	Keynote 1:	**Mark A. Reed**, Yale University
		Nanofluidic Ionic Devices
09:45 -10:10	Invited 1:	**Zhenyu Zhang,** University of Science and Technology of China
		Crossing over from three-dimensional nonequilibrium growth to two-dimensional van der Waals epitaxy
10:10 -10:35	AoE 1:	**Fei Liu,** The University of Hong Kong
		Cold Source Transistor: Energy Efficient Switching by Source Density of States Engineering
10:35 - 11:00 Tea Break		
Chairperson: Prof. Jiannong Wang Hong Kong University of Science and Technology		
11:00 - 11:45	Keynote 2:	**Thomas Szkopek**, McGill University
		Device Engineering with 2D Materials
11:45 -12:10	Invited 2:	**Lan Chen**, Institute of Microelectronics, Chinese Academy of Sciences
		The Modeling Technologies for Design and Manufacture Co-optimization
12:10 - 14:00 Lunch Break		
Chairperson: Prof. Jian Wang, HKU		
14:00 - 14:45	Keynote 3:	**Enge Wang**, Chinese Academy of Sciences
		Full quantum nature of interfacial water
14:45 - 15:10	Invited 3:	**Lvzhou Li**, Sun Yat-sen University
		当大数据遇到量子计算---谈谈量子算法
15:10 - 15:35	AoE 2:	**Wang Yao**, The University of Hong Kong
		Spintronics in the moire
15:35 - 16:00 Tea Break		
Chairperson: Prof. Zhenyu Zhang, USTC		
16:00 - 16:25	Invited 4:	**Tai Min**, Xi'an Jiaotong University
		Interfacial Magnetism and Its Application to STT-MRAM
16:25 -16:50	Invited 5:	**Yan Zhou**, The Chinese University of Hong Kong, Shenzhen
		Magnetic Skyrmions in Nanostructures
18:00 - 21:00	Banquet	

Tuesday, October 16, 2018		
Chairperson: Prof. Tai Min, XJTU		
09:00 - 09:25	Invited 6	**Xuefeng Guo,** Peking University
		Carbon Electrode-Molecule Junctions: A Reliable Platform for Molecular Electronics
09:25 - 09:50	AoE 3	**Qin Liu,** The University of Hong Kong
		Computational Methodologies for Heterogeneous Electromagnetic Systems
09:50 -10:15	AoE 4	**Mansun Chan**, Hong Kong University of Science and Technology
		i-MOS: a Cloud Based Circuit Simulation and Compact Modelling Platform
10:15 - 10:40 Tea Break		
Chairperson: Prof. Keli Wu, The Chinese University of Hong Kong		
10:40 - 11:05	Invited 7:	**Jinfeng Kang**, Peking University
		Non-volatile Memory Based Computing Paradigms for High-Efficiency Data Processing
11:05 - 11:30	AoE 5:	**Hong Guo**, HKU&McGill
		Computational Materials Science by RESCU - a KS-DFT Method for Solving Thousands of Atoms
11:30 - 11:45	Closing Remarks **Fuchun Zhang**， The University of Hong Kong & University of Chinese Academy of Sciences	
11:45 - 14:00 Lunch Break		
14:00 - 15:00	Free Discussion	
15:00 - 18:00	Hiking	

Keynote Speech 1:

Nanofluidic Ionic Devices



Mark A. Reed *[1], Sylvia Xin Li[1], and Weihua Guan[2]

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[2]Pennsylvania State University, State College, PA 16801

Abstract:

Solid-state nanofluidic devices have proven to be ideal systems for studying the physics of ionic transport at the nanometer length scale. When the geometrical confining size of fluids approaches the ionic Debye screening length, a number of new transport phenomena occur, which have wide ranging implications to diverse areas such as biological ion channels, desalination, and energy storage and conversion. We have demonstrated a variety of nanofluidic ionic devices which utilize controllable ion selectivity, allowing us to realize ionic diodes and field effect transistors.[1] These devices have remarkable analogies to their semiconductor counterparts, but with some important differences.

One of the most intriguing implications of nanofluidic ionics is the ability to construct artificial ion channels. We have demonstrated[2] that we can create membrane potentials similar to cellular systems, with the additional ability to tune the ion selectivity ratio. The detailed dynamics of the transport allows us to identify relevant relaxation times and mechanisms, which could enable engineering of faster ionic and neural systems.

The study of nanofluidic ionic systems has primarily used monovalent ion

systems. However, divalent ions comprise some of the most important ion channels in biological systems. We have investigated divalent nanofluidic ion transport, and have observed charge inversion at the channel/fluid interface.[3] The observation of charge inversion has important implications to the theory of a strongly correlated liquid (SCL) and biological permselectivity.

Finally, we will show some implications and applications. There are a number of naturally occurring systems which utilizes this physics for permselective ion transport, and engineered nanofluidic batteries. We observe an unexpected improvement of electrochemical performance in a nanofluidic battery, with important implications for increased energy storage.

References:

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Invited Speech 1:

Crossing Over from Three-dimensional Nonequilibrium Growth to Two-dimensional Van der Waals Epitaxy

Zhenyu Zhang*

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Abstract:

This talk will focus on demonstrating how to apply what we learned in three-dimensional nonequilibrium growth to gaining a better understanding of the atomistic mechanisms in van der Waals epitaxy of two-dimensional systems as we attempt to optimize the functionalities of such materials.

AOE Speech 1:

Cold Source Transistor: Enegy Efficient Swtihcing by Source Density of States Engineering

Fei Liu *[1], Jian Wang[1] and Hong Guo[1,2]

[1] AoE & Department of Physics, The University of Hong Kong, Hong Kong, China
*[2] Centre for the Physics of Materials & Department of Physics, McGill University, Montreal, Canada. *E-mail: feiliu@hku.hk*

Abstract:

Achieving sub-60 mV/decade FET switching is critical for reducing power dissipation in integrated circuits. In this talk, I will present our recent work in realizing a new steep slope FET by source density of state engineering, named as cold source transistor. The cold source suppresses "hot" electrons at the thermal tail of the source's Fermi distribution and benefits sub-60 mV/decade switching. I will discuss the design considerations of cold source more generally and show sub-60 mV/decade switching by: (i) using gapless graphene as injection source and, (ii) introducing a band gap in the source where a p-type Si, a thin metal and a n-type Si are combined to form the cold source of Si FET. The feasibility, design consideration and optimization of the cold source FET will be discussed.

Keynote Speech 2:

Device Engineering with 2D Materials

Thomas Szkopek*

Department of Electrical and Computer Engineering, McGill University, Montreal, Canada.
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Abstract:

The current renaissance of interest in layered materials, especially in monolayer form, has created new opportunities for electronic device engineering. An important observation is that the semi-metallic nature of graphene has limited its use in both digital and analog transistor applications. We have nonetheless experimentally demonstrated that large area graphene field effect transistors can be used for ion-sensing with a detection limit on par with spectroscopic titration. High performance is achieved by saturating both thermodynamic and quantum capacitance limits in sensing layer design, while making use of low-flicker noise in large-area devices. In the digital domain, we argue that aggressively scaled graphene nanomechanical switches could achieve steep slope operation by making use of the low flexural rigidity of graphene and the exponential scaling of tunneling current. Finally, we note that less well known 2D materials have bandstructures well suited to device engineering. One such example is the monochalcogenide SnSe, whose quasi-2D bandstructure realizes a Hicks-Dresselhaus thermoelectric.

Invited 2:

The Modeling Technologies for Design and Manufacture Co-optimization

Lan Chen*

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Abstract:

Chemical mechanical planarization(CMP) is one of the most important step during IC manufacture, which is used to remove redundant materials and to keep the surface of chips and wafer flatten. When CMOS processing technologies come into 14nm and beyond, both the HKMG and FinFET devices need CMP to process the metal gate. Right now, the CMP processing is not only effects the parasitic RC characters of interconnect lines but also devices' characters. The lecture will introduce our research work on how to building a CMP model and how to use the model to co-optimize with the design patterns to get a better manufacturability. We proposed here is a kind of manufacture aware design methodology, which is also called DTCO by Synopsys. This methodology can also expand its application into MEMS、flash et al areas.

Keywords:

Chemical Mechaincal Planarization(CMP), process variation, design pattern, design and manufacture co-optimization.

Keynote Speech 3:

Full Quantum Nature of Interfacial Water

Enge Wang*[1,2]

[1]International Center for Quantum Materials and School of Physics, Peking University

*[2]Institute of Physics, Chinese Academy of Sciences. *E-mail: egwang@iphy.ac.cn*

Abstract:

Water-solid interactions are of broad importance in nature and technology. Using a combination of experimental (cryogenic STM) and theoretical (first-principle electronic structures and molecular dynamics) methods, we systematically studied the full quantum nature of water on salt surface. These results shed light on our understanding of water-solid interactions, which would be helpful in designing novel water/solid interface structures and utilizing such structures for the study of water clustering and concerted proton tunneling in more complicated systems.

Invited Speech 3:

当大数据遇到量子计算---谈谈量子算法

Lvzhou Li*

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Abstract:

随着大数据时代的到来，发展适用于大数据环境的新算法和新模型成为信息领域面临的重要课题。而量子计算由于强大的信息存储能力和计算上的并行性使其具有应对大数据问题的天然基因。然而，量子计算潜在的并行性并非直接可以利用的，而是需要根据所解决的问题经过巧妙的算法设计才可能。因此，要充分发挥出量子计算的潜能，能否设计出快速的量子算法是关键。本报告首先将指出量子计算并行性的原理所在，然后回顾量子算法的发展过程，着重介绍量子算法近期的一些重要进展，特别是解线性方程组的对数时间量子算法及其应用，以及量子机器学习算法等。这些最新进展预示着量子计算在大数据处理和人工智能领域具有巨大的应用潜能。

AoE Speech 2:

Spintronics in the Moire

Wang Yao*

*Department of Physics, The University of Hong Kong. *E-mail: wangyao@hku.hk*

Abstract:

Van der Waals stacking of the 2D semiconductors into vertical heterostructures is a powerful approach towards designer quantum materials that can combine and extend the exotic properties of the building blocks. Ubiquitous to these vdW heterostructures is the formation of moiré pattern due to the inevitable lattice mismatch. We show that the moiré offers unprecedented opportunities for nanoscale patterning of electronic, optical and topological properties. We will also discuss moire effects in 2D magnets, which can lead to formation of skrymions.

Invited Speech 4:

Interfacial Magnetism and Its Application to STT-MRAM

Tai Min

Center for Spintronics and Quantum Systems, School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China.
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Abstract:

Interfacial spintronics has gain great attentions recently for its rich physical phenomenon associated with spin-orbit coupling and intrinsic symmetry breaking. Recent discoveries of interface-induced magnetism and noncollinear spin textures, nonlinear dynamics including spin-transfer torque, spin-orbit torque and magnetization reversal induced by interfaces have made this field exiting and fast growing. One of practical applications of interace spintronics is the successful development and commercialization of Spin-Transfer-Torque Magnetic Random Access Memory (STT-MRAM) as one of the next generation of mainstream nonvolatile memories. Recently, our studies have found that under a small electric bias voltage, the exchang coupling of synthetic anti-ferromagnetic multilayer system can be changed between an anti-ferromagnetic coupling state and a ferromagnetic coupling state. Based on this phenomenon, a new type of STT-MRAM was proposed and of which the critical switching current can be reduced by an assisting electric field, especially at sub-nano-second region. Micromagnetic simulation has been performed to study the switching behavior of the magnetization of the synthetic anti-ferromagnet free layer with tunable Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction under the impact of the electric field.

Invited Speech 5:

Magnetic Skyrmions in Nanostructures

Yan Zhou*

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Abstract:

In this talk, I will present some of our recent work on micromagnetics simulations of magnetic skyrmions in constricted geometries. We propose some new mechanisms for skyrmion creation and manipulation in nanostructures such as nanowires and nanodisk. We believe our study is fundamentally important for a better understanding of how to inject and control skyrmions as information carriers in nanoscale hybrid spintronic and magnonic devices.

Invited Speech 6:

Carbon Electrode-Molecule Junctions: A Reliable Platform for Molecular Electronics

Xuefeng Guo*

*College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P.R. China. *E-mail : guoxf@pku.edu.cn*

Abstract:

This talk will exemplify our on-going interest and great effort in developing efficient lithographic methodologies capable of creating molecular electronic devices through the combination of top-down micro/nanofabrication with bottom-up molecular assembly. These devices use nanogapped carbon nanomaterials (such as single-walled carbon nanotubes (SWCNTs) and graphene) as point contacts formed by electron beam lithography and precise oxygen plasma etching. Through robust amide linkages, functional molecular bridges terminated with diamine moieties are covalently wired into the carboxylic acid-functionalized nanogaps to form stable carbon electrode-molecule junctions with desired functionalities. We have used these approaches to reveal the dependence of the charge transport of individual metallo-DNA duplexes on p-stacking integrity, and fabricate molecular devices capable of realizing label-free, real-time electrical detection of biological interactions at the single-event level, or switching their molecular conductance upon exposure to external stimuli, such as ion, pH and light.

References

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Invited Speech 7:

Non-volatile Memory Based Computing Paradigms for High-Efficiency Data Processing

JinFeng. Kang*, P. Huang, R.Z. Han, Y.C. Xiang, C. Liu, Y.N. Jiang, Z. Zhou, L.F. Liu, and X.Y. Liu,

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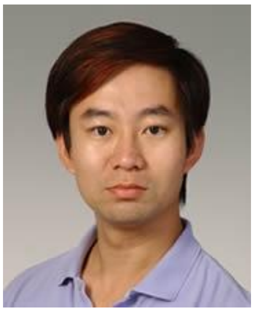
Abstract:

With the development of new information technologies such as AI, IOT, Big Data etc., the data deluge era is coming. It is required to process the high volume of and non-structured data in high-efficiency and smart ways. Meanwhile, the CMOS scaling is approaching the fundamental limits and the traditional processor architecture is suffering from the so-called von Neumann Bottleneck. Therefore, it is imperative to innovate new computing paradigms beyond traditional von Neumann approach. In this talk, the NVM-based novel computing paradigms beyond traditional processor architecture are presented. In the new computing paradigms, non-volatile memory devices such as Flash and Resistive-switching random access memory (RRAM) are used to build the hardware architecture implementations to achieve high efficiency of data processing. Regarding to the specific application scenarios, the newly developed computing paradigms based on NVM devices demonstrate the excellent computing power.

AOE Speech 4:

i-MOS: a Cloud-based Circuit Simulation and Compact Modeling Platform



Lining Zhang and **Mansun Chan***

Dept. of ECE, Hong Kong University of Science & Technology,
*Clear Water Bay, Kowloon, Hong Kong. *Email:* mchan@ust.hk

Abstract:

In this presentation, we will provide and update of the development of the interactive Modeling and Inline Simulation (i-MOS) platform which provides online simulation interface for a wide collection of emerging devices. Since the launch of i-MOS in 2013, there are already 18 device models implemented with more than 700 users. Recent developments including the implementation of the Artificial Neural Network Model, the dynamic time evaluation simulation approach and Jacobian matrix reduction by internal node removal techniques. The deployment of the circuit simulation user interface and integration of ab initio simulation modules will also be explained. Through the various collaboration efforts, i-MOS has already become one of the hubs for model developers and early technology adopters to interact.

AOE Speech 5:

Computational Materials Science by RESCU - a KS-DFT Method for Solving Thousands of Atoms

Hong Guo*[1,2]

[1] AoE & Department of Physics, The University of Hong Kong, Hong Kong, China
*[2] Centre for the Physics of Materials & Department of Physics, McGill University, Montreal, Canada. *E-mail: hong.guo@mcgill.ca*

Abstract:

A major stumbling block for solving realistic materials problems is the lack of a first principles method that can accurately, efficiently and comfortably calculate condensed phase materials comprising thousands of atoms. Solving large systems is necessary when dealing with materials involving interfaces, surfaces, dilute impurities, grain boundaries, dislocations, magnetic domains, solvents, bio-materials etc. Well known Kohn–Sham density functional theory (KS-DFT) solvers can solve problems at a few hundred atoms level on modest computer hardware. For larger systems, further approximations are typically applied at the expense of accuracy.

In this talk I shall discuss our effort in developing a powerful general-purpose KS-DFT solver called RESCU – stands for Real space Electronic Structure CalcUlator. We demonstrate that RESCU can compute electronic structure for systems comprising many thousands of atoms on modest computer resources, for metals, semiconductors, insulators, DNA-in-water, Moire patterns in 2D heterojunctions, dilute doped III-nitrides, etc. RESCU achieves high efficiency without compromising accuracy. For these problems and up to 14,000 atoms, RESCU converges KS-DFT in a few to ten wall-clock hours. I shall discuss the novel computational mathematics behind the

efficiency gain and present several materials physics examples solved by RESCU.

Acknowledgements: I thank Dr. Vincent Michaud-Rioux who is the main developer of RESCU. Several others contributed important works: Dr. Lei Zhang for forces and relaxation, Ying-Chin Chen for HSE06 and GW, Dr. Saeed Bohloul for DFPT, Dr. Xiaobin Chen for phonon. I wish to thank many other researchers who helped us improving the RESCU.