

Session 24: Modeling and Simulation - 2D Materials, Modeling, and the Optimization of Beta-Ga2O3 Power Devices

Tuesday, December 4, 2:15 PM

Plaza A

Co-Chairs: R. Williams, IBM

M. Pala, University of Paris-Saclay

2:20 PM - 2:45 PM

24.1 Interfacial Thermal Conductivity of 2D Layered Materials: An Atomistic Approach, *K. Parto, A. Pal, X. Xie, W. Cao and K. Banerjee, University of California, Santa Barbara*

This paper presents the first comprehensive modeling and analysis of thermal transport across both lateral and vertical interfaces to two-dimensional (2D) layered materials. Using an ab-initio atomistic Green's function approach that accurately accounts for the interface geometry including the van der Waals gap, as well as interatomic force constants and interface phonon scatterings, we provide estimation of crucial interfacial thermal properties including thermal conductivity that are invaluable for assessing the performance, scaling, and reliability limits of all emerging 2D based nano-devices, interconnects, circuits and non-planar (monolithic 3D) integration schemes.

2:45 PM - 3:10 PM

24.2 Computational Design of Silicon Contacts on 2D Transition-Metal Dichalcogenides: The Roles of Crystalline Orientation, Doping Level, Passivation and Interfacial Layer, *X. Ma, Z. Fan*, J. Wu, X. Jiang*, J. Chen, University, Qingdao, *Chinese Academy of Sciences*

Systematic numerical simulations based on density functional theory (DFT) and non-equilibrium Green's function (NEGF) formalism have been carried out for comprehensive understanding of the physical properties of silicon contacts on monolayer transition metal dichalcogenides (TMDs). The effects of different contact crystalline orientations including Si (001), (110) and (111), silicon doping levels, possible surface passivation such as H- and F-, as well as interfacial layer (IL) engineering using BN and Graphene are thoroughly discussed. On the one hand, it was found that the contact properties of different crystalline orientations follow similar trend, and the doping modulation of the Schottky barrier height (SBH) remains inappreciable in a practical range of doping level. On the other hand, H- and F- passivation are found to be effective ways to diverge the intrinsic contact into n- and p- type contacts, respectively. In addition, monolayer BN as IL was found to form surprisingly good p-type contact with vanishing p-SBH.

3:10 PM - 3:35 PM

24.3 First Principles Study of Memory Selectors using Heterojunctions of 2D Layered Materials, *L. Li, B. Magyari-Köpe*, C.-H. Wang*, S. Deshmukh*, Z. Jiang*, H. Li*, Y. Yang, H. Li, H. Tian, E. Pop*, T.-L. Ren, H.-S. Philip Wong*, Tsinghua University, *Stanford University*

Two-dimensional (2D) tunnel heterojunctions with an H-shaped energy barrier could serve as ultrathin memory selectors with good symmetry, non-linearity, and high endurance. Atomically thin 2D layered materials can potentially deliver high on-state tunneling current density. We explore the design space for H-shaped memory selectors using heterojunctions of 2D layered materials, using physical modeling and first principles density functional theory (DFT) quantum transport simulations. The difference between simulations and the few existing experiments is also discussed. A selector must be designed to suit the resistive memory (1R) characteristics. We evaluate the H-shaped selector in the one-selector-one-resistor (1S1R) configuration and provide design guidelines for the heterojunction (metal/nL hBN/nL 2D material/nL hBN/metal) design to match with the 1R characteristics.

3:35 PM

Coffee Break

4:00 PM - 4:25 PM

24.4 Can Kinetic Inductance in Low-Dimensional Materials Enable a New Generation of RF-Electronics?, *K. Agashiwala, A. Pal, W. Cao, J. Jiang and K. Banerjee, University of California, Santa Barbara*

Kinetic Inductance has been recently exploited at room temperature to create materials with inductance densities that exceed the traditional Faraday limit. In this work, for the first time, we develop a rigorous theoretical framework to uncover the physics and origin of kinetic inductance to identify/engineer the materials for addressing inductance-density and performance requirements in next generation passive devices for RF-ICs. Employing three different approaches (Drude model, Fermi sphere and the Boltzmann Transport Equation), we provide guidelines for optimally exploiting kinetic inductance in natural as well as engineered low-dimensional materials to simultaneously achieve maximum inductance-density and performance required for next-generation RF/wireless applications.

4:25 PM - 4:50 PM

24.5 A Surface Potential- and Physics- Based Compact Model for 2D Polycrystalline-MoS₂ FET with Resistive Switching Behavior in Neuromorphic Computing, *L. Wang, L. Wang, K.-W. Ang, A. Voon-Yew Thean, G. Liang, National University of Singapore*

For the first time, a surface potential- and physics-based compact model for two dimensional (2D) polycrystalline- molybdenum disulfide (MoS₂) field effect transistors (FETs) with resistive switching (RS) behavior is developed and verified by experimental data. This model is incorporated with the theories of thermal activation transport, grain boundary (GB) barrier and space charge limited current (SCLC). Based on the GB induced disorders, the grain size, low temperature, and high electrical field dependent characteristics are studied. The predicted transfer and output characteristics have an excellent quantitative agreement with experimental results. Furthermore, considering the hopping process induced defect- (i.e., sulfur vacancy) redistribution, the GB (e.g., intersecting or bisecting GB) dependent resistive switching behavior is physically investigated. Finally, this model is implemented to simulate the synaptic activity such as short-term/long-term plasticity, which indicates the possibility of using 2D-FETs for neuromorphic computing applications.

4:50 PM - 5:15 PM

24.6 Design and Optimization of β -Ga₂O₃ on (h-BN layered) Sapphire for High Efficiency Power Transistors: A Device-Circuit-Package Perspective, *B. K. Mahajan, Y.-P. Chen, W. Ahn, N. Zagni and M. Ashraful Alam, Purdue University*

Despite exceeding the Baliga's Figure of Merit (BFOM) by 400% and Huang's Chip Area Manufacturing FOM (HCAFOM) by 330% [1], the performance of existing β -Ga₂O₃ FETs is inferior to that of GaN, primarily due to extreme self-heating. Self-heating effect (SHE) has emerged as an important concern for device performance, output power density, run-time variability and reliability for modern logic transistors. The effects are even more severe for high-power transistor where the channel material may be a poor thermal conductor, e.g. β -Ga₂O₃. Very high internal electric fields, extreme temperature and mechanical stresses associated with these transistors drive electrochemical reactions [2], influence atomic processes [3], and accelerate multiple non-equilibrium effects [4]. A device-circuit-package, multi-physics, multi-scale simulation is needed to capture these effects self-consistently, but such a model has not yet been developed. In this paper, we (i) develop the first self-consistent device (TCAD), circuit (HSPICE), and package (COMSOL) model considering SHE which predicts FET performance on variety of substrates accurately; (ii) use the model to propose a novel hexagonal-Boron Nitride (h-BN) based β -Ga₂O₃ FET with 30% (cf. Sapphire substrate) and 80% (cf. SiO₂ substrate) reduction in thermal resistance (R_{th}); (iii) demonstrate the performance of boost converter (with parameters extracted from our TCAD model) with

h-BN based β -Ga₂O₃ FET, which outperforms the existing β -Ga₂O₃ FETs, achieving an efficiency within 10-15% of highest performing enhancement mode (E-mode) GaN FET; (iv) propose h-BN based FinFET which exceeds the ION of the existing β -Ga₂O₃ FET by more than 500%; and (v) develop a Faraday-cage type novel packaging strategy for effective heat dissipation and efficient system performance in β -Ga₂O₃ FETs.