Session 24 - Modeling and Simulation - Ab Initio Simulation of Materials, Devices, and Interconnects
Tuesday, December 10, 2:15 p.m.
Continental Ballroom 7-9
Co-Chairs: B. Magyari-Kope, TSMC
V. Georgiev, University of Glasgow

2:20 PM **24.1** First-Principles Parameter-Free Modeling of n- and p-FET Hot-Carrier Degradation
Markus Jech, Stanislav Tyaginov, Ben Kaczer, Jacopo Franco, Dominic Jabs, Christoph Jungemann, Michael Waltl, Tibor Grasser, TU Wien, imec, RWTH Aachen University

We present and validate a quantum chemistry approach to capture the intricate nature of hot-carrier degradation, which is essentially free of fit parameters. The newly identified resonance scattering mechanism allows us to clearly reveal the differences between degradation in n- and p-channel devices.

2:45 PM **24.2** Computational Study of Spin Injection in 2D Materials
Arnab Pal, Kamyar Parto Kunjesh Agashiwala, Wei Cao, Kaustav Banerjee, University of California, Santa Barbara

This work presents the first comprehensive study of spin-injection into 2D materials using ab-initio Density Functional Theory simulations coupled with Non-Equilibrium-Greens-Function formalism, for applications in both spintronics and Magnetic Tunnel Junctions. Our rigorous modeling and simulation framework provide important insights into the relatively unexplored phenomenon of spin-injection into 2D-material systems.

3:10 PM **24.3** Ab initio Simulation of Advanced Materials and Devices: Current Challenges (Invited)
Philippe Blaise, Silvaco Montbonnot, CEA-Leti

By integrating atomistic tools into the catalogues of TCAD solution providers, simulation is going to take the next step. First, we describe the most promising strategy of atomistic tools usage. Then, we open up new perspectives due to the strong link between electronic devices variability and atomistic modeling.

3:35 PM *COFFEE BREAK*

4:00 PM **24.4** *Ab initio* Mobility of Single-layer MoS_2 and WS_2: Comparison to Experiments and Impact on the Device Characteristics
Youseung Lee, Sara Fiore, Mathieu Luisier, ETH-Zurich

We combine the linearized Boltzmann Transport Equation and quantum transport by means of the Non-equilibrium Green's Functions to simulate monolayer MoS_2 and WS_2 ultra-scaled transistors with carrier mobilities extracted from experiments. Electron-phonon, charged impurity, and surface optical phonon scattering are taken into account from ab initio calculations or measurements.

4:25 PM **24.5** Piezoelectric Hetero-junction Tunnel FET with Staggered Gap at off-state and Broken Gap at on-state
Yuxiong Long, Hong-Yu Wen, Shenyuan Yang, Jun Huang, Xiangwei Jiang, Institute of Semiconductors, Chinese Academy of Sciences, MaxLinear Inc.

A novel GaSb/InAs piezoelectric hetero-junction tunnel-FET (PE-H-TFET) which changes band-gap type during switching is proposed, i.e. staggered-gap at OFF-state while broken-gap at ON-state. Numerical simulation suggests that the PE-H-TFET achieves 1.76 times enhancement of I_{ON} and a steep SS of 42 mV/decade. The source overlap obtains 2.5 times I_{ON} enhancement.

4:50 PM **24.6** Large-scale *ab initio* Quantum Transport Simulation of Nanosized Copper Interconnects: the Effects of Defects and Quantum Interferences

Meng Ye, Xiangwei Jiang, Shu-Shen Li, Lin-Wang Wang, Chinese Academy of Sciences, Lawrence Berkeley National Laboratory

A fully ab initio quantum transport simulation of nano-interconnect containing record number of atoms (~5000) is presented for the first time. Various imperfections of the nanosized Cu interconnects are thoroughly investigated. It is suggested that classical description, e.g. Matthiessen's rule, is not valid at nanoscale, due to quantum interference.