

Thursday Morning, August 6, 2026

International Workshop on Gallium Oxide and Related Materials (IWGO-6)

Room ESJ 0202 - Session IWGO-ThM1

Theory, Modeling, and Simulation

Moderators: Jinwoo Hwang, The Ohio State University, Joel Varley, Lawrence Livermore National Laboratory

8:00am IWGO-ThM1-1 Breakfast

8:30am IWGO-ThM1-7 Impact of Defects and Impurities on the Properties of Al₂O₃, Chris G. van de Walle, UCSB INVITED

Aluminum oxide (Al₂O₃) has a broad range of applications. Alloys of Al₂O₃ and Ga₂O₃ of course also serve as barrier layers in heterojunctions for Ga₂O₃-based devices. In metal-oxide-semiconductor (MOS) technologies, it can be used as a high-k gate dielectric, to passivate the surface of Si substrates, or as the tunneling layer of non-volatile flash memory devices. Al₂O₃ is also frequently used in superconducting qubits, as a tunneling barrier in the Josephson junction and/or as a substrate and capacitor dielectric.

Defects in the oxide layer affect the performance, for instance by leading to changes in threshold voltage. In quantum applications, the qubits are sensitive to defects in the substrate or in the tunnel barrier of the Josephson junction. Dielectric loss can also lead to decoherence. Enhanced control over devices thus requires a thorough understanding of the structural, electronic, and optical properties of potential defects and impurities.

We have performed first-principles calculations to elucidate these issues. For point defects, we focused on the dominant species, which are the oxygen and aluminum vacancies, and provided detailed characterization of their optical properties, which can aid experimental observation and identification [1]. For dielectric loss, we focused on mechanisms that could affect coherence at the operating frequencies of superconducting qubits, which are around about 5 GHz. We identified a mechanism by which charged defects or impurities can absorb electromagnetic radiation at GHz frequencies by emission of acoustic phonons [2]. Finally, for donor impurities, we have complemented our study of Si [3] with a comprehensive study of alternative impurities in both the corundum and monoclinic phase of Al₂O₃, identifying candidate dopants that are remarkably shallow in light of the very large band gap of this material.

Work performed in collaboration with J. L. Lyons, S. Mu, Y. Shin, S. Mu, M. Turiansky, J. B. Varley, H. Wang, M. Wang, D. Wickramaratne, and C. Wilhelmer, and supported by DOE, ONR and AFOSR.

[1] C. Wilhelmer, M. E. Turiansky, D. Waldh r, L. Cvitkovich, C. G. Van de Walle, and T. Grasser, *Phys. Rev. Mater.* **9**, 096202 (2025).

[2] M. E. Turiansky and C. G. Van de Walle, *APL Quantum* **1**, 026114 (2024).

[3] S. Mu, M. Wang, J. B. Varley, J. L. Lyons, D. Wickramaratne, and C. G. Van de Walle, *Phys. Rev. B* **105**, 155201 (2022).

8:55am IWGO-ThM1-12 GeO₂ and Ge_xSn_{1-x}O₂ Alloys: Emerging Ultra-Wide-Band-Gap Materials for Power Electronics, Emmanouil (Manos) Kioupakis, University of Michigan, Ann Arbor INVITED

In this talk, I will present recent advances by my research group, our collaborators, and the broader community on rutile GeO₂ and its alloys with SnO₂, a new UWBG semiconductor materials platform for power electronics. I will survey our first-principles investigations of the thermodynamic stability, electronic structure, defect physics, carrier transport, and thermal properties of rutile GeO₂ and Ge_xSn_{1-x}O₂ alloys. Complementing the theoretical insights, I will highlight recent experimental progress from our collaborators on the synthesis and characterization of GeO₂-based materials. These results provide critical validation of theoretical predictions and shed light on the practical challenges associated with materials quality and phase stability. Moreover, I will provide a brief overview of broader efforts by the global research community on rutile GeO₂ and its alloys SnO₂, spanning different growth techniques, doping strategies, and characterization approaches. This perspective will help identify key bottlenecks and opportunities for advancing these materials toward device applications.

9:20am IWGO-ThM1-17 Rutile Ge_xSn_{1-x}O₂ Alloys for Ultra-Wide Bandgap Electronics: Phase Stability and Bandgap Engineering, Alp Kurbay, University of Michigan, Ann Arbor; Yann M ller, EPFL, Switzerland; Xiao Zhang, University of Michigan, Ann Arbor; Anirudh Natarajan, EPFL, Switzerland; Emmanouil Kioupakis, University of Michigan, Ann Arbor

Ge_xSn_{1-x}O₂ alloys have recently attracted attention as candidate ultra-wide bandgap (UWBG) materials for power electronics due to their predicted ambipolar dopability, high carrier mobilities, and high thermal conductivity. Experiments show that these alloys can be grown as thin films over a wide composition range, have carrier mobilities that are insensitive to alloy disorder at low Ge content, and exhibit breakdown fields as high as 7.0 ± 1.4 MV/cm [1]. In this study, we perform a comprehensive investigation of the thermodynamic stability, structural parameters, and electronic properties of Ge_xSn_{1-x}O₂ alloys using first-principles atomistic calculations. The large positive mixing enthalpy produces a miscibility gap with a critical temperature above 2300 K, which agrees with the experimental phase diagram for bulk materials [2]. This indicates that the high solubilities observed in thin-film synthesis cannot be explained by the incoherent phase diagram alone. We demonstrate that coherency strain during epitaxial growth substantially alters phase stability, and calculations of the coherent spinodal show significant suppression of the miscibility gap, reducing the critical temperature to ≈ 900 K. Our calculations show that these alloys exhibit only weak short-range order, with a slight tendency for Ge-Sn nearest-neighbor clustering, and can be approximated as random solid solutions. Our calculated lattice parameters exhibit a nearly linear dependence on composition, consistent with Vegard's law and experimental measurements. Hybrid-functional calculations show a direct band gap at the Γ -point ranging from ~ 3.6 eV in SnO₂ to ~ 4.7 eV in GeO₂ with strong compositional bowing and light carrier effective masses. The calculated bandgaps in the Sn-rich region show a ~ 200 meV difference between thin films and bulk alloys, and we explore possible causes such as compressive strain and interfacial effects from the substrates. Our results reveal the thermodynamic origin of the metastability of Ge_xSn_{1-x}O₂ thin films and demonstrate the potential of this system for band-gap engineering in ultra-wide-bandgap oxide semiconductors [3].

[1] U. Mansur et al., *Phys. Status Solidi A*, 202501029 (2026).

[2] Watanabe, *J. Am. Ceram. Soc.* **66**, c104 (1983).

[3] M ller et al., arXiv:2601.12184, <https://doi.org/10.48550/arXiv.2601.12184>.

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9:35am IWGO-ThM1-20 Single Ga-Layer Reconstruction Mediates Ga₂O₃ Heteroepitaxy: A Multiscale Atomistic Study, Ilaria Bertoni, Aldo Ugoletti, Anna Marzegalli, Universita' degli Studi di Milano-Bicocca, Italy; Flyura Djurabekova, University of Helsinki, Finland; Leonida Miglio, Universita' degli Studi di Milano-Bicocca, Italy

Ga₂O₃ heteroepitaxy on c-plane sapphire displays a rich polymorphic competition, with different phases stabilizing depending on growth conditions [1]. Under high-temperature/ low-rate conditions—approaching quasi-equilibrium growth—largely relaxed β -Ga₂O₃ crystallites grow on sapphire, often mediated by a thin α wetting layer at the interface [2]. The coherent β /substrate interface is characterized by a strongly anisotropic mismatch strain, as large as $\sim 9\%$ along one of the two in-plane directions, thus making the observed stabilization of β without classical misfit dislocations particularly remarkable. The thermodynamic and atomistic mechanism behind this α/β sequence remains poorly understood.

Through a multiscale framework combining density functional theory, classical nucleation theory and continuum elasticity modeling, we show that α wetting of sapphire is thermodynamically driven by surface energetics, justifying the formation of a thin α interlayer of up to ~ 3 bilayers. Beyond this thickness, a crossover emerges: three-dimensional β islands, relaxing elastically through their free surfaces, become thermodynamically favored above a critical size, providing a purely thermodynamic rationale for the experimentally observed $\alpha \rightarrow \beta$ sequence.

Moreover, upon thermal activation, molecular dynamics simulations reveal a collective atomic rearrangement at the β/α interface that goes well beyond elastic relaxation, enabling near-complete strain release. This plastic reconstruction is confined to a single Ga atomic plane: as the β island expands toward its bulk lattice parameter, at the interface the relaxed β oxygen sublattice periodically overlaps with different sites of the underlying strained α sublattice, causing the interfacial Ga layer to respond to the local oxygen-sublattice environment by adopting an α -like or β -like coordination within the same atomic plane. The oxygen framework remains

perfectly crystalline across the interface, with strain accommodated entirely via this cation redistribution — a mechanism fundamentally distinct from dislocation-mediated relaxation.

This interfacial plasticity provides a permanent, size-independent strain-relief pathway that explains how β -Ga₂O₃ can stabilize on a strained α wetting layer even after island coalescence, consistent with experimental observations under quasi-equilibrium growth conditions.

[1] ACS Appl. Mater. Interfaces 17, 62261–62276 (2025)

[2] Applied Physics Express 8, 011101 (2015)

9:50am **IWGO-ThM1-23 Carrier Mobility in Ge_xSn_{1-x}O₂ Alloys from First Principles, Amanda Wang, Alp Kurbay, Xiao Zhang, Nick Pant, Emmanouil Kioupakis**, University of Michigan

SnO₂ and GeO₂ are both transparent conducting oxides in the rutile crystal structure, with band gaps of 3.6 eV and 4.7 eV, respectively. Alloying the two enables tunability of the band gap and of the lattice constants, as well as potential for ambipolar doping due to the predicted ambipolar dopability of GeO₂. However, a shortcoming of many semiconductor alloys is that the disordered potential landscape caused by the random arrangement of atoms results in carrier scattering, impeding mobility. Despite this, experiments have found high electron mobilities in Ge_xSn_{1-x}O₂ alloys that are insensitive to alloy composition, indicating a lack of alloy scattering [1,2]. In this work, we calculate the electron and hole mobilities in Ge_xSn_{1-x}O₂ alloys using first-principles electronic structure methods to predict the theoretical upper limit of mobility and examine the role of alloy scattering across the composition range. The carrier mobility limited by phonon- and ionized-impurity scattering is calculated for the binary end compounds, in good agreement with experimental measurements for SnO₂. To characterize the alloy scattering, we model random alloys using supercells and perform slab calculations to align the band edges across the composition range. The alloy scattering is combined with the phonon- and ionized-impurity scattering to determine the total alloy mobility. We find that the insensitivity of the band edges with respect to composition results in weak alloy scattering and high electron mobilities that are invariant to composition, especially in the range of low Ge composition, reproducing the trend from experiments as seen in Figure 1. This confirms that Ge_xSn_{1-x}O₂ alloys are promising wide-band-gap semiconductors with efficient carrier transport.

[1] Y. Nagashima, *et al.*, Chem. Mater. 34(24), 10842–10848 (2022).

[2] H. Takane, *et al.*, Phys. Rev. Mater. 6(8), 084604 (2022).

10:05am **IWGO-ThM1-26 A Novel Vertical β -Ga₂O₃ Transistor Architecture Without Planarization or Mid-Gap Acceptor Blocking Layers, Akilesh Srikanth**, The Ohio State University; Siddharth Rajan, Ohio State University

We report on the Isolated Source Electrode Field Effect Transistor (ISEFET) - a new vertical β -Ga₂O₃ transistor architecture that can be fabricated without planarization or ion implanted acceptor-based current blocking layers (CBL). Due to the absence of p-type doping, vertical Gallium Oxide devices must be fabricated using either a vertical Fin/Trench-MOSFET [1-3] or UMOSFET [4,5]/CAVET [6] topologies. Vertical FINFETs require multiple planarization and precision etch processes to successfully produce a working device. UMOSFETs require current blocking layers using mid-gap acceptors which degrade transport and lead to trapping effects. Here we show successful demonstration of a novel device architecture that avoids the use of both planarization and ion implanted mid-gap acceptors. The fabrication process flow for this transistor requires one sub-micron feature definition with a self-aligned deep etch, and no additional critical alignment steps, making it suitable for rapid prototyping and large-scale manufacturing of future Gallium Oxide and other wide bandgap semiconductor transistors.

These ISEFETs were fabricated on HVPE-grown (001) β -Ga₂O₃ Sn-doped conductive substrates (NCT inc., 10 μ m [Si] $\sim 10^{16}$ cm⁻³). An n^+ source contact layer with target depth of 150nm and concentration of 5×10^{19} cm⁻³ was formed through a multi-energy Si ion implantation. The dielectric CBLs were then formed using PECVD SiO₂, followed by fin source metallization (Ti/Au/Ni) using E-Beam Lithography and SBP metallization. Self-aligned fins were etched using ICP/RIE, followed by PEALD Al₂O₃. Gate metallization (Ni/Au) was done through e-beam evaporation and DC sputtering. Then deposited backside drain contact (Ti/Au) and opened source bond pads using RIE etching.

The measured results from the highest aspect ratio multi-fin devices had a fin width of 0.2 μ m and fin height of 1.2 μ m with a threshold voltage $V_{TH} = 1$ V and $I_{ON}:I_{OFF}$ ratio of 10⁷. The measured breakdown voltage $V_{BR} = 500$ V and $R_{ON} = 676$ m Ω -cm². The highest obtained output current density was

$I_D \sim 70$ A/cm² at $V_D = 10$ V, $V_G = 15$ V for lower aspect ratio structures. The high on-resistance in this first-generation device is attributed to incomplete activation and/or degradation of the ion-implanted contact layer. Further improvements in R_{ON} and V_{BR} can be made in the next generation of devices by optimizing the n^+ activation conditions, post-etch damage recovery, and adding effective field management strategies. The demonstration of this new device architecture - isolated source field effect transistor (ISEFET) – provides a promising path for future development and manufacturing of high power vertical transistors based on β -Ga₂O₃.

Author Index

Bold page numbers indicate presenter

— B —

Bertoni, Ilaria: IWGO-ThM1-20, **1**

— D —

Djurabekova, Flyura: IWGO-ThM1-20, **1**

— K —

Kioupakis, Emmanouil: IWGO-ThM1-17, **1**;
IWGO-ThM1-23, **2**

Kioupakis, Emmanouil (Manos): IWGO-
ThM1-12, **1**

Kurbay, Alp: IWGO-ThM1-17, **1**; IWGO-
ThM1-23, **2**

— M —

Marzegalli, Anna: IWGO-ThM1-20, **1**

Miglio, Leonida: IWGO-ThM1-20, **1**

Müller, Yann: IWGO-ThM1-17, **1**

— N —

Natarajan, Anirudh: IWGO-ThM1-17, **1**

— P —

Pant, Nick: IWGO-ThM1-23, **2**

— R —

Rajan, Siddharth: IWGO-ThM1-26, **2**

— S —

Srikanth, Akilesh: IWGO-ThM1-26, **2**

— U —

Ugolotti, Aldo: IWGO-ThM1-20, **1**

— V —

van de Walle, Chris G.: IWGO-ThM1-7, **1**

— W —

Wang, Amanda: IWGO-ThM1-23, **2**

— Z —

Zhang, Xiao: IWGO-ThM1-17, **1**; IWGO-
ThM1-23, **2**