

## DS 11: Focus Session: Quantum Properties at Functional Oxide Interfaces 1 (joint session HL/DS)

Modern oxide materials exhibit a rich variety of physical properties that lead to potential applications such as sensors and detectors, solar energy harvesting, transparent and power electronics. Understanding their quantum properties at surfaces and interfaces may play a decisive role for functionalities in high-electron-mobility transistors, quantum electronics or topological quantum computation. These typically require homo- or heteroepitaxial layers of high crystallinity and investigation methods designed to reveal the fascinating physics at (complex) oxide interfaces. This session sets a focus on growth of oxide interfaces, the experimental and theoretical investigation of their novel physical, in particular quantum properties as well as fabrication and characterization of demonstrator devices.

Organized by Martin Albrecht, Oliver Bierwagen, and Saskia F. Fischer

Time: Tuesday 9:30–12:45

Location: H34

**Invited Talk** DS 11.1 Tue 9:30 H34  
**Materials and Device Engineering for Gallium Oxide-based Electronics** — NIDHIN KURIAN KALARICKAL<sup>1</sup>, SUSHOVAN DHARA<sup>1</sup>, ASHOK DHEENAN<sup>1</sup>, and ●SIDDHARTH RAJAN<sup>1,2</sup> — <sup>1</sup>ECE Department, The Ohio State University — <sup>2</sup>MSE Department, The Ohio State University

This presentation will discuss our recent work on epitaxy, heterostructure design, and electrostatics to achieve high-performance  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> lateral and vertical electronic devices. We will discuss some key results in materials growth and device design for lateral structures, including the first  $\beta$ -(Al,Ga)<sub>2</sub>O<sub>3</sub>/ $\beta$ -Ga<sub>2</sub>O<sub>3</sub> modulation-doped structures with excellent transport properties, double-heterostructure modulation-doped structures, and scaled delta-doped transistors with cutoff frequency of 27 GHz, and self-aligned lateral field effect transistors with > 900 mA/mm current density. We will discuss the use of a new damage-free epitaxial etching technique using Ga atomic flux that enables highly precise fabrication of 3-dimensional structures, and applications of this etching to realize field termination in vertical diodes, and lateral FINFETs with enhanced performance. Extreme-permittivity dielectrics provide unique opportunities to create devices that can sustain extreme fields without premature breakdown of metal-semiconductor and dielectric-semiconductor interfaces. We will discuss promising results of electrostatic engineering using BaTiO<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub> heterojunctions that enable high fields to be sustained within Gallium Oxide diodes and transistors.

**Invited Talk** DS 11.2 Tue 10:00 H34  
**Ferroelectric two-dimensional electron gases for oxide spin-orbitronics** — ●JULIEN BRÉHIN — Unité Mixte de Physique CNRS/Thales

Just as the apparent incompatibility between ferroelectricity and magnetism prompted the renaissance of multiferroics, the research on ferroelectric metals conjectured in the 1960s by Anderson and Blount was recently revitalized. Yet, their experimental demonstration remains very challenging due to the contra-indication between the presence of free charge carriers and switchable electric dipoles. In this talk we will report on two-dimensional electron gases (2DEGs) formed on Ca-substituted SrTiO<sub>3</sub> (STO). Signatures of the ferroelectric phase transition near 30 K are visible in the temperature dependence of the sheet resistance RS and in a strong, reproducible hysteresis of RS with gate voltage. In addition, spectroscopic measurements of the 2DEG region indicate the presence of switchable ionic displacements. Beyond their fundamental interest in materials physics, ferroelectric 2DEGs offer opportunities in spin-orbitronics: we will show how their spin-charge conversion properties, caused by the inverse Rashba-Edelstein effect, can be electrically tuned in amplitude and sign in a non-volatile way. These results open the way to a whole new class of ultralow-power spin-orbitronic devices operating without the need for magnetization switching. Finally, we will describe how one can introduce magnetism into such systems to achieve multiferroic 2DEGs displaying magneto-electric coupling.

DS 11.3 Tue 10:30 H34  
**Electron transport of the two-dimensional electron gas in polar-discontinuity doped LaInO<sub>3</sub>/BaSnO<sub>3</sub> heterostructure** — GEORG HOFFMANN<sup>1</sup>, FAZEEL ZOHAI<sup>1</sup>, MARTINA ZUPANCIC<sup>2</sup>, MARTIN ALBRECHT<sup>2</sup>, and ●OLIVER BIERWAGEN<sup>1</sup> — <sup>1</sup>Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, D-10117 Berlin, Germany —

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Transparent semiconducting oxides (TSOs) are key players for new (opto-)electronic devices and two-dimensional electron gases (2DEGs) are relevant for high-frequency applications. Polar-discontinuity doping (interfacing a polar material with a nonpolar one), has been demonstrated to provide a 2DEG at the interface between the perovskites LaAlO<sub>3</sub> and SrTiO<sub>3</sub> with a high electron concentration but suffers from low room-temperature (RT) electron mobilities of SrTiO<sub>3</sub>. In this contribution we demonstrate polar-discontinuity doped 2DEG at the interface between the perovskites LaInO<sub>3</sub> and BaSnO<sub>3</sub>, grown by plasma-assisted molecular beam epitaxy. While the individual, undoped oxide layers were found to be insulating, the formation of the polar-discontinuity doped 2DEG at their interface is confirmed by capacitance-voltage (CV) and van der Pauw-Hall measurements. The extracted sheet electron concentrations >2e13cm<sup>-2</sup> and RT electron mobilities above >50cm<sup>2</sup>/Vs are promising for device applications. The transport properties of the 2DEG are compared to those of L-doped BaSnO<sub>3</sub> layers.

DS 11.4 Tue 10:45 H34  
**Non-Abelian braiding of phonons in monolayer oxides** — ●BO PENG<sup>1</sup>, ADRIEN BOUHON<sup>1</sup>, BARTOMEU MONSERRAT<sup>1,2</sup>, and ROBERT-JAN SLAGER<sup>1</sup> — <sup>1</sup>TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — <sup>2</sup>Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom

Non-Abelian braiding of quasiparticles can encode quantum information immune from environmental noise with the potential to realize topological quantum computation. Here we propose that phonons, a bosonic excitation of lattice vibrations, can carry non-Abelian charges in their band structures that can be braided using external stimuli. Taking some earthly abundant materials such as silicates [1] and aluminium oxide [2] as representative examples, we demonstrate that an external electric field or electrostatic doping can give rise to phonon band inversions that induce the redistribution of non-Abelian charges, leading to non-Abelian braiding of phonons. We show that phonons can be a primary platform to study non-Abelian braiding in the reciprocal space, and we expand the toolset to study such braiding processes.

References: [1] Bo Peng, Adrien Bouhon, Bartomeu Monserrat & Robert-Jan Slager. Nature Communications 13, 423 (2022). [2] Bo Peng, Adrien Bouhon, Robert-Jan Slager & Bartomeu Monserrat. Physical Review B 105, 085115 (2022).

**30 min. break**

DS 11.5 Tue 11:30 H34  
**Shift of the absorption onset in corundum-like  $\alpha$ -(Ti<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub>** — ●ELIAS KLUTH<sup>1</sup>, MICHAEL FAY<sup>2</sup>, CHRISTOPHER PARMENTER<sup>3</sup>, JOSEPH ROBERTS<sup>4</sup>, FABIEN MASSABUAU<sup>5</sup>, RÜDIGER GOLDHAHN<sup>1</sup>, and MARTIN FENEBERG<sup>1</sup> — <sup>1</sup>Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — <sup>2</sup>Advanced Materials Research Group, Faculty of Engineering, University of Nottingham, NG7 2RD, UK — <sup>3</sup>Nottingham Nanotechnology and Nanoscience Centre, University of Nottingham, University Park, Nottingham NG7 2RD, UK — <sup>4</sup>School of Engineering, The University of Liverpool, Liverpool L69 3GH, UK — <sup>5</sup>Department of Physics, SUPA, University of

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Corundum-like  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> is a metastable phase of the polymorphic ultra-wide band gap semiconductor Ga<sub>2</sub>O<sub>3</sub>. While previous research has mostly focused on the stable  $\beta$ -phase the  $\alpha$ -phase is less discussed, but interesting as well as it allows bandgap-engineering by alloying e.g. with  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (sapphire) or In<sub>2</sub>O<sub>3</sub>.

Since the transition metal oxide Ti<sub>2</sub>O<sub>3</sub> as well, has a corundum-like phase ( $\alpha$ -phase), with a small lattice mismatch of about 3.5% to  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub>, we investigate here (0001)  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> thin films alloyed with Ti, grown by ALD (atomic layer deposition).

We use spectroscopic ellipsometry in ultraviolet range to obtain the complex dielectric function (DF) of  $\alpha$ -(Ti<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> up to  $x = 0.61$ . We find a clear red shift of the absorption onset with increasing Ti content, as well as an increase of the amplitude of the DF.

DS 11.6 Tue 11:45 H34

**Optical signatures of polarons trapped at ferroelectric domain walls in bismuth ferrite** — ●SABINE KÖRBEL — Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — Friedrich Schiller University Jena, Germany

Ferroelectric domain walls are atomically narrow planes that can behave very differently from the surrounding bulk ferroelectric material. For example, the domain walls in many ferroelectrics can collect and conduct charge carriers despite the insulating nature of the host material. Domain walls can be created, moved, and removed again in a controlled way, thus they can be used to alter the electronic properties of the ferroelectric as desired. Charge carriers that accumulate at domain walls may induce metallic or semiconducting behavior depending on whether they are delocalized or form self-trapped small polarons. The latter may be detected, for example, as deep levels within the band gap in absorption or photoluminescence spectra. Here we predict optical signatures of charge carriers trapped as small polarons at ferroelectric domain walls in BiFeO<sub>3</sub>, using first principles calculations.

DS 11.7 Tue 12:00 H34

**Anharmonicity of lattice vibrations in  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> investigated by temperature dependent Raman spectroscopy** — ●JONA GRÜMBEL<sup>1</sup>, RÜDIGER GOLDHAHN<sup>1</sup>, DAE-WOO JEON<sup>2</sup>, and MARTIN

FENEBERG<sup>1</sup> — <sup>1</sup>Otto-von-Guericke Universität, Magdeburg, Germany — <sup>2</sup>Korea Institute of Ceramic Engineering and Technology, Jinju, Republic of Korea

We investigate the Raman excitations of a corundum-like  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> thin film under temperature variation from 80K up to 790K. This yields detailed information about anharmonic processes in the crystal. For the two dominant phonon modes for each of the two Raman-active phonon mode symmetries ( $A_{1g}$  and  $E_g$ ) model calculations are performed in order to quantify the contributions of different decay mechanisms. It is shown, that our experimental data can be well described by the applied theoretical models. The determined coefficients of cubic and quartic decay for both, phonon energy and linewidth, are compared with those from hexagonal GaN and AlN as well as with those from  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>. We observe, that for the two selected phonon modes of  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> the quartic decay processes are negligible for the phonon frequencies, but not for the phonon linewidths behavior under temperature variation. A quantitative description within the model parameters is presented.

**Invited Talk**

DS 11.8 Tue 12:15 H34

**Strain-driven dissociation of water on (incipient) ferroelectrics** — JOSHUA L. BATES and ●CHIARA GATTINONI — Department of Chemical and Energy Engineering, London South Bank University, London, UK

Functional materials have great promise in catalysis, and especially within dynamic catalytic cycles, where the “functional” properties are used to cyclically modify the local environment of a surface to enhance turnover frequency. In particular, strain-driven mechanisms exploiting the properties of piezo- and ferroelectric materials, are of great interest.

In this work we focus on (incipient) ferroelectric nanomaterials BiFeO<sub>3</sub>, BaTiO<sub>3</sub>, KTaO<sub>3</sub> and SrTiO<sub>3</sub>, perovskites presenting a wide range of bulk properties and behaviours. We uncover how interplay between these properties (such as the spontaneous polarization) and nanoscale effects (such as the depolarizing field and the surface structure), affect the strain-driven water-splitting abilities of these nanoscale functional materials. Finally, we identify the most desirable properties for a highly efficient ferroelectric material for dynamic catalysis.