HL 52: Oxide Semiconductors II

Time: Thursday 15:00–17:15 Location: H14

HL 52.1 Thu 15:00 H14

Connection between electronic structure and crystal symmetry in bismuth vanadate — •Philip Schwinghammer, Franziska Hegner, Frederico Delgado, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

The electronic and structural properties of bismuth vanadate (BVO) were characterized using density functional theory (DFT). Previous work in the literature indicated that semi-local exchange was incapable of correctly reproducing the ground-state structure of BVO, but disagreed on which functional would improve the description. We found that the Heyd-Scuseria-Ernzerhof hybrid functional could accurately predict the monoclinic ground state structure, provided spin-orbit coupling was included. Semi-local density functionals mischaracterize the hybridization of the lone pair Bi6s states and O2p states near the valence band edge, which is corrected by hybrid functionals. Due to the large mass of bismuth, spin-orbit coupling is required for an accurate description of the electronic structure. When both corrections are taken into account, we find that the valence and conduction band edges in BVO are extremely flat, leading to large effective masses along one direction in reciprocal space. The effective carrier masses are affected by the ionic structure, indicating a possible reason for the different photo-catalytic efficiencies of tetragonal and monoclinic scheelite BVO.

HL 52.2 Thu 15:15 H14

Blue shift of the absorption onset and bandgap bowing in rutile $Ge_xSn_{1-x}O_2$ — •Elias Kluth[1], Yo Nagashima[2], Shohei Osawa[3], Yasushi Hirose[3], Jürgen Bläsing[1], André Strittmatter[1], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany — [2]Department of Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo, Tokyo, 113-0033, Japan — [3]Department of Chemistry, Tokyo Metropolitan University, 1-1 Minamiosawa Hachioji, Tokyo 192-0397, Japan

Rutile-GeO_2 has recently attracted increasing research interest as an ultra wide bandgap oxide similar to Ga_2O_3 with the unique advantage that theoretical calculations predict the possibility of ambipolar doping. In contrast rutile-SnO_2 is a well-established transparent conductive oxide (TCO) widely used in solar cells and displays. Alloying SnO_2 with Ge offers a promising pathway to developing deep ultraviolet (DUV) TCOs. However, investigations into the optical properties of the $Ge_xSn_{1-x}O_2$ system remain limited.

In this study, we employed spectroscopic ellipsometry in the visible and ultraviolet region to determine the ordinary dielectric functions of $Ge_xSn_{1-x}O_2$ thin films grown by pulsed laser deposition (PLD) on rutile-TiO_2 substrates. Our analysis reveals a systematic blue shift of the onset of absorption with increasing Ge content. By evaluating the dielectric functions, we extracted the characteristic transition energies at the absorption onset and determined the bowing parameter of the dipole-allowed direct bandgap to be $b = 0.70$ eV.

HL 52.3 Thu 15:30 H14

$NaNbO_3$, $KNbO_3$, and their solid solutions: A *first-principles* and special quasirandom structures investigation — •Daniel Fritsch — Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany — University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Germany

Ferroelectric materials crystallising in the perovskite structure, like $NaNbO_3$ and $KNbO_3$, have come into focus as lead-free and environmentally friendly alternatives to the widely used piezoelectric ceramic $Pb[Zr_xTi_{1-x}]O_3$ (PZT) [1].

They both exhibit a large range of structural phase transitions and accompanying changes in their ferroelectric behaviour. While the material properties of both end members are relatively well known, this is much less the case for their solid solutions.

Here, we present results for $Na_{1-x}K_xNbO_3$ solid solutions based on *first-principles* calculations for the structural and electronic properties, and so-called special quasirandom structures to investigate the solid solutions [2]. The obtained results will be compared to available experimental findings and other theoretical investigations.

[1] D. Fritsch, Adv. Mater. Sci. Eng. **2018**, 6416057 (2018).

[2] D. Fritsch, Appl. Sci. **12**, 2576 (2022), J. Phys. Condens. Matter **36**, 375702 (2024).

HL 52.4 Thu 15:45 H14

Spintronic properties of the two-dimensional electron gas in KTaO3-based heterostructures. — •Sonali Kakkar[1] and Chandan Bera[2] — [1]Department of Physics, Noida Institute of Engineering and Technology, 19, Institutional Area, Knowledge Park II, Greater Noida, Uttar Pradesh 201306, India — [2]Institute of Nano Science and Technology, Sector-81, Knowledge City, Sahibzada Ajit Singh Nagar, Punjab, 140306, India

A two-dimensional electron gas (2DEG) in oxide interfaces offers a single platform for a wide range of functionalities. Compared to STO-based 3d-2DEG, 2DEG in the polar perovskite oxide KTaO3 (KTO) with 5d-t2g orbitals shows a greater atomic spin-orbit coupling. Moreover, the electronic and spintronic properties of oxide heterostructures are greatly influenced by the inherent crystal structure symmetry. In this work, we have investigated the electronic and spintronic properties in KTO-based heterostructures using density functional theory calculations with the Hubbard parameter (DFT+U). The dependence of the Rashba spin-splitting and the corresponding spin texture in the reciprocal space for 2DEG at the KTO surface and LVO/KTO interface on the crystal orientation highlights the importance of crystal symmetry for the 5d-2DEG in KTO [1]. Furthermore, highly confined, spin-polarized 2DEG at the interfacial TaO2 layer in the 5dxy orbitals of Ta at the interface between the ferromagnetic insulator EuO and the non-magnetic KTO shows Rashba spin texture [2]. [1] S. Kakkar, et al., Physica E Low Dimens. Syst. Nanostruct. 144, 115394 (2022). [2] S. Kakkar, et al., Adv. Phys. Res. 2, 2200026 (2023).

15 min. break

HL 52.5 Thu 16:15 H14

Unraveling the mechanism of resistive switching in titanate-based perovskites — Wahib Aggoune[1,2], •Parrydeep Kaur Sachdeva[1], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195, Berlin, Germany — [2]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Memristors capable of switching between high and low resistance states while retaining memory, hold promise for non-volatile memory. A recent fascinating experimental work observed high resistive switching (RS) in *off*-stoichiometric paraelectric titanate-based perovskites $ATiO_3$ (A=Sr, Ca) [1]. It suggests that RS is driven by defects, though their exact role remains unclear. Here, we investigate the defects behavior using density functional theory. Under the experimental growth conditions, the complex defect (Ti-interstitial with *A*-vacancies) is thermodynamically stable, pinning the Fermi level close the conduction band. Remarkably, the *off*-center shift of the interstitial atom induces a local polarization and gives rise to localized mid-gap states. Switching between the equivalent *off*-center sites faces energy barriers of 0.1–0.8 eV, depending on the pathway. This switches both polarization direction and the defect charge distribution. Therefore, upon applying a voltage, the overall polarization driven by the local shifts of the defects can be switched. As this also redistributes the defect charge states, it switches the resistance state. Our findings provide insights into the origin of RS toward memristor development.

[1] A. Baki, *et al.*, *Sci. Rep.*, **11**, 7497 (2021).

HL 52.6 Thu 16:30 H14

Ultraviolet Emission from $^6P_{7/2}$ Stark Manifold in Gd-Implanted β-Ga_2O_3 Thin Films — •Martin S. Williams[1,2], Mahmoud Elhajhasan[1], Marco Schowalter[1], Lewis Penman[3], Alexander Karg[1], Fabien C.-P. Massabuau[3], Andreas Rosenauer[1], Gordon Callsen[1], Carsten Ronning[4], Martin Eickhoff[1,2], and Manuel Alonso-Orts[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliothekstraße 1, 28359 Bremen, Germany — [3]Department of Physics, SUPA, University of Strathclyde, Glasgow, United Kingdom — [4]Institute of Solid State Physics, Friedrich-Schiller-University Jena, Helmholtzweg 3, 07743 Jena, Germany

Monoclinic gallium oxide (β-Ga$_2$O$_3$) is a promising ultra-wide band gap semiconductor for the next generation of optoelectronic devices. Despite its attractive material properties, its luminescence spectrum is dominated by defect emission in the visible spectral range and a dominating UV emission in β-Ga$_2$O$_3$ has rarely been observed. An enhancement of the UV emission in β-Ga$_2$O$_3$ by optically active ion doping in β-Ga$_2$O$_3$ is only achieved with gadolinium (Gd^{3+}).

In this work, β-Ga$_2$O$_3$ thin films grown by molecular beam epitaxy and atomic layer deposition are implanted with Gd and thermally activated. Four separate luminescence peaks, from the Stark-split ^{6}P$_{7/2} \rightarrow {}^8$S$_{7/2}$ transition in Gd^{3+}, are individually resolved with linewidth $\leq$ 2 meV. The influence of growth technique, implantation parameters and annealing temperature is investigated.

HL 52.7 Thu 16:45 H14

Investigation of the bond length dependence and lattice relaxation in zincblende Cu(Br,I) alloys — •Sandra Montag[1], Stefan Merker[2], Michael Bar[1], Richard J. Schenk[1], Eva Zollner[1], Konrad Ritter[1], Timo Pfeiffelmann[1], Sergiu Levcenko[1], Edmund Welter[3], Holger von Wenckstern[1], Marius Grundmann[1], Harald Krautscheid[2], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Institute of Inorganic Chemistry and Crystallography, Leipzig University, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

CuI is a promising p-type wide-bandgap semiconductor with various applications in the field of transparent electronics. Among the numerous doping and alloying candidates, the Cu(Br,I) alloy system offers the opportunity to tailor the free hole concentration in functional layers, enabling optimized performance of active devices, such as pn-diodes and transistors. Using X-ray absorption spectroscopy, the fine structure of CuBr$_{1-x}$I$_x$ powder and thin film samples, with anion composition x varying from 0 to 1, was measured. The analysis of the extended fine structure reveals a nonlinear change of the Cu-Br and Cu-I bond lengths with composition x. This behaviour is different from that reported for III-V and II-VI zincblende alloys, but comparable to the rocksalt RbBr$_{1-x}$I$_x$ alloy. The observed bond length bowing may therefore be a characteristic feature of group I-VII alloys. To uncover the degree of lattice relaxation with increasing distance from the absorbing atom, the higher neigbour scattering signal is evaluated.

HL 52.8 Thu 17:00 H14

Revealing the incorporation site and local structure of Ni and Se in doped CuI thin films — •Mustafa G. Yazlak[1], Christiane Dethloff[1], Philipp Storm[1], Michael Lorenz[1], Sandra Montag[1], Hans H. Falk[1], Edmund Welter[2], Sofie Vogt[1], Marius Grundmann[1], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

This study investigates polycrystalline CuI thin films with varying nickel (Ni) and selenium (Se) concentrations, grown on glass substrates using Pulsed Laser Deposition (PLD) and co-sputtering. CuI:Ni thin films, with 1*30 at% Ni and thicknesses between 0.1*1.0 μm, and CuI:Se thin films, with 0.4*3.8 at% Se and $\sim$1.0 μm thickness, were prepared and capped with Al$_2$O$_3$ layers to prevent oxidation. X-ray Absorption Spectroscopy (XAS) at low temperatures ($\sim$10 K) was conducted at the Cu, Se, and Ni K-edges to study the local structure of Ni and Se in the CuI matrix. The near edge structure and extended fine structure for a pure CuI thin film at the Cu K-edge suggests possible Cu oxidation. For CuI:Ni thin films, an increase in Ni concentration correlates with reduced Cu oxidation because Ni prefers to bond with oxygen rather than iodine, forming disordered NiO as seen from the Ni K-edge spectra. For CuI:Se thin films, the Cu K-edge spectra show small changes but no clear trend with Se content and the Se K-edge spectra indicate a Cu neighborhood similar to Cu$_2$Se and CuSe. Quantitative analyses are in progress to provide a deeper understanding of how Ni and Se content affects local structural changes.