# Final report for projects funded by the Leibniz Association's Competition Procedures

Reporting period: July 1, 2020 — December 31, 2024

**Project title: GraFOx2**

**Project number: W40/2019**

## Executive Summary

In its second funding period, the LeibnizScience Campus "Growth and fundamentals of oxides for electronic applications", GraFOx II, builds on the successful fundamental materials research of GraFOx I and expands it towards device related work and data science. To this end, two extra-university institutes (HZB and FBH) and two universities (Leipzig and Magdeburg) have joined as full partners. GraFOx structures its work in four clusters, spanning the entire range from materials exploration in "Cluster X" to the processing and investigation of devices based on matured materials in "Cluster D". The growth (Cluster "G") and physical properties activities (Cluster "P") support and strongly interact with both X and D. Each cluster comprises several coordinated projects.

The project`s start was constrained by significant budget cuts at Leibniz Association and by COVID restrictions that hindered meetings and experimental work in year one. Partners mitigated these impacts through institutional co-funding > 9 Mio € in competitive awards from DFG, BMBF and the Leibniz Association. Expanded use of video conferences enabled regular seminars with international speakers as well as a summer school with international participation during the pandemic.

Device-oriented highlights include BMBF-funded work on vertical power devices involving, IKZ, PDI, and HZB, and a strong focus on materials for neuromorphic computing (IKZ, HZB). Materials breakthroughs include Czochralski growth of highly-doped 2 inch $Ga_2O_3$ bulk,[1] MOCVD growth of $Ga_2O_3$ at high growth rates,[2] and first vertical normally-off power devices demonstrating a field strength of 3MV/cm.[3] In novel materials, world record room temperature electron mobilities were achieved for two-dimensional electron gases at epitaxially engineered $BaSnO_3/LaInO_3$ interfaces,[4] and flux-grown bulk Sb-doped rutile $GeO_2$ has been demonstrated as a promising power-electronics semiconductor that hold the promise for p-doping and therefore could outperform $Ga_2O_3$.[5] From a properties and theory perspective, a fully anharmonic nonperturbative theory of vibronic band structure renormalization[6] explains the experimentally measured temperature dependence of the bandgap of Perovskites measured within GraFOx. Additionally, a parameter free approach to compute oxide-surface free energies both rationalized an experimentally observed surface reconstruction and will guide future $Ga_2O_3$ growth modeling.[7] Extensive, reproducible growth and characterization of sesquioxides polytypes was pursued across several partners and includes international collaborations.[8–14]

GraFOx partners (HU, FHI, IKZ, PDI, and Leipzig University), playing a leading role in the project FAIRmat, advancing a federated data infrastructure for materials science. International cooperation expanded through joint projects with the universities of Parma, Michigan, Seoul National University, and Cornell University. Recognition of Grayfox's impact includes the Leibniz chair for Darell Schlom and a Humboldt Research Award for Kookrin Char from Seoul University. Training outcomes strong: 20 PhD and 16 master theses were finalized accompanied by 40 peer reviewed publications by PhD students in the reporting period. A community highlight was the 5$^{th}$ edition of the IWGO in Berlin which attracted 219 participants from 24 countries.

Successful activities of GraFOx are continuing in multiple smaller scale and network projects on national and EU level both, already running and applied for.

# 1. Achievement of objectives and milestones

The following list refers to milestones and deliverables defined in the proposal (see GraFOx_II_Milestones.pdf).

### Milestones

- M1.1—M2 have been reached
- M3 has not been reached: Not all PhD positions could be filled (see "2. Activties…")
- M4.1—4 have been reached: 2 Focus sessions held/organized for virtual Fall meeting 2021 and 2022 meeting, since 2023 "Oxide semiconductors" became regular sessions with large GraFOx participation
- M5.1 has not been reached: The planned student training seminar has not been conducted due to Covid.
- M6 has been reached: An international online Summer School "Oxides for Electronic Applications" co-organized by GraFOx and IKZ has been run in August 16-18, 2021.
- M7 has been reached: WGO 2024 was successfully held in Berlin (https://grafox2022.pdi-berlin.de/iwgo-2024/)
- M8 has been reached: Due to the COVID pandemic no conferences have been conducted until 2021. from 2022 on, GraFOx shaped the oxide-related program of ICMBE 2022 and 2024, as well as IWGO 2022, and conducted international workshops.
- M9.1/2: has not been reached: Due to the COVID pandemic no outreach activities have been conducted until 2022,
- M9.3/4: has been reached: Since then, GraFOx students were involved in "Berlin science week" 2023, 2024 and Girls day, and PDI hosted an artist in residence in 2024
- M10 has been reached: Concepts to continue GraFOx are being actively pursued (see 8. Outlook).
- MX1 has been reached: Phase diagrams for $(In,Ga)_2O_3$,[15] $(Al,Ga)_2O_3$,[14] $(Ti,Ga)_2O_3$,[16]
- MX2 has been reached using kappa-$(Al,Ga)_2O_3$/$(In,Ga)_2O_3$[11] heterostructures
- MX3 has been reached: [17]
- MG1 has been reached: [1]
- MG2 has been reached, to be published
- MG3 has been reached: [18]
- MP1 has been reached: [19]
- MP2 has been reached: [6]
- MP3 has been reached for $Ga_2O_3$ (presented at IWGO 2024, to be published), for $SrTiO_3$ had already been published by another group[20]
- MD1 has been reached: [3]
- MD2 has not been reached due to so far limited layer thickness
- MD3 has not reached
- MD4 has not reached (related DFG proposal to fund project D5 rejected)

### Deliverables

- D1.1/D2.1 Midterm reports to advisory board and Leibniz sent in 2022
- D1.2/2.2 Activity now documented on our webpage, D2.2 is the present report
- D4/D5.1-2 20 PhD theses finished; 16 Bachelor/Master theses finished
- D6.1 40 peer-reviewed publications by GraFOx PhD students
- D7.1 24 publications were joint work of multiple GraFOx partner institutions
- D8.1 >50 presentations by PhD students at international conferences
- D9.1 >30 invited presentations at international conferences

### Financial statement/planning

A 25% budget reduction applied to all Leibniz ScienceCampi in the 2020 call severely affected the start of GraFOx II. To preserve the full workplan and task scope, we eliminated the speaker's budget (€65,000) and reduced personnel costs by €235,000. Networking activities

formerly covered by the speaker's budget are now partially financed by the extra-university institutes IKZ, HZB, FBH and PDI. Following the Fritz-Haber-Institute´s withdrawal from the GraFOx II cooperation agreement in June 2021, the financial and personnel resources (1 PhD position) were transferred to Humboldt University.
Personnel expenditures were below planned for the reporting period. Budget personnel costs were €289,450 for year 1, and €317,950 for year 2; actual personnel spending through December 2021 totaled €237,248.98. The underspend is primarily due to the midyear project start (July 2020), COVID-19 related hiring delays, and temporary vacancies in PhD positions (see obstacles in next section).

## 2. Activities and obstacles

### Activities

of GraFOx cover the following categories:

(1) Research in GraFOx II is organized into four clusters that together span the full research and development chain, from early materials discovery to device demonstration. Cluster X focuses on materials exploration, Cluster G on growth and synthesis, Cluster P on physical property characterization, and Cluster D on the processing and investigation of devices based on matured materials. Because G (growth) and "P" (physical properties) support all material systems, they interact intensively with X and D. Each cluster comprises several projects; a typical project is led by a single partner and staffed by one PhD student or postdoc, as detailed in the attached project list. Projects supported by third party funding are likewise assigned to the relevant clusters and labeled accordingly. During the reporting period, the Leibniz ScienceCampus hosted 33 projects in total (see GraFOx_II_Project_List.pdf), conducted by 18 PhD students, 7 Postdocs, and 8 scientists, advised by 20 PIs. The research program centers on two main materials thrusts: (i) binary oxides- most notably $Ga_2O_3$, now sufficiently mature for device processing and investigation, and the novel rutile-$GeO_2$ which has the potential to outperform $Ga_2O_3$ – (i) complex oxides, including semiconducting $SrTiO_3$, $BaSnO_3$ in combination with dielectric $LaInO_3$ and ferroelectric $(K,Na)NbO_3$. Work proceeds both within the individual cluster projects in the clusters and through cross-cutting focus topics that link multiple projects and clusters.

(2) Scientific exchange, conducted through topical meetings on focus topics, regular online GraFOx seminars (with internal and external international speakers), online/hybrid GraFOx meetings, and the (co)organization of symposia at international conferences.

(3) Student training. Delivered within individual projects, and through seminars, project meetings with poster presentations, and the international summer school (Milestone M6).

(4) Dissemination. Achieved primarily via publication in international, peer-reviewed journals, books and book chapters, and presentations at international conferences and workshops.

(5) Project coordination and acquisition (more details below and under 5. Structure and Collaboration) as will be detailed below.

### Obstacles

encountered were twofold:

1) The 25% reduction in Leibniz funding for GraFOx had a strong negative impact on the co-funding and on funding new PhD positions. To accomplish the projects tasks all partners agreed to limit the funding for PhD positions to 32 months, with the expectation institutional funds would cover the remainder. Subsequentially, several university partners were unable to close this gap to the extent that research organizations as Helmholtz, Leibniz and Max-Planck could. This lead either to unfilled PhD positions or to the tradeoff of hiring postdocs for shorter

terms. Part of the short fall has since been mitigated by third party funding from DFG, BMBF and Leibniz.
2) The COVID-19 pandemic had significant consequences. In-person meetings were reduced to a minimum, which was particularly challenging for newly hired PhDs and Postdocs. Conference travel was largely impossible, limiting international exchange and reducing the visibility of PhDs and Postdocs. Widespread restriction on laboratory work also impeded Master´s theses making recruitment into PhD positions exceptionally difficult. Relocation of hired PhD students and postdocs from abroad to Germany were delayed by up to 18 months. Newly established online formats during the COVID alleviated these issues by enabling intensified the international cooperation, short notice invitations of international speakers, and organization of schools with broad international participation.

### Advances in the field

Applications for $Ga_2O_3$ devices have progressed to the development of vertical high-power devices. Key challenges include the availability of highly conducting bulk substrates, achieving high growth rates for the active zone, and maintaining low well controlled n-type doping while preserving high mobility. First normally-off devices have been demonstrated; although *p*-type doping in $Ga_2O_3$ remains elusive, this gap is mitigated by employing *p*-type oxides (e.g. NiO) in hetero-*pn* junctions for rectification and field management. Substrate sizes of $Ga_2O_3$ continue to scale with 4” wafers commercially available and 6” demonstrated. In parallel bandgap engineering via alloying with $Al_2O_3$ has increased the effective bandgap while retaining *n*-type semiconducting behavior. These topics are being addressed by GraFOx partners IKZ, FBH, HZB and PDI in larger projects in cooperation with industry that leverage state of the art machine learning approaches and using the profound experience in materials development that has been established within GraFOx I. A promising ultra-wide bandgap semiconductor, rutile $GeO_2$, has been theoretically predicted to outperform $Ga_2O_3$. Motivated by this, we initiated growth and characterization efforts under Leibniz-funding within a collaborative project. In addition, neuromorphic device concepts crucial for energy efficient AI hardware are advancing worldwide. Building on biga big data based approaches which have been developed at FHI, the partners FHI, IKZ and Humboldt-Universität zu Berlin are pursuing materials by design strategies. The combination of excellence in synthesis, computation and data science within this Leibniz funded effort is unique and hold the promise for a successful outcome of this project.

## 3. Results and successes

Since GraFOx is a research and training campus, our primary output are peer reviewed publications and the development of early career researchers. During the reporting period we produced more than110 peer-reviewed publications in international journals, including >20 joint publications co-authored by multiple GraFOx partners and more than 40 publications with external partners featuring GraFOx co-authors. These publications underscore both the internal cohesion of the campus and its integration into the global scientific community.
Training outcomes are equally strong. 18 PhD students and 2 students were directly involved into GraFOx’ projects. In addition 16 finished Bachelor/Master theses, and 20 finished doctoral dissertations were completed, and our PhD students served as first authors on 40 publications – clear evidence of GraFOx´ s rolein fostering scientific independence and visibility. GraFOx also succeeded in attracting substantial external support: 9 Mio € in third party funding was secured for 17 new projects launched during GraFOx II, spanning collaborative research initiatives as well as a dedicated science communication project.

## 4. Equal opportunities, career development and internationalization

We are committed to advancing women´s careers in science. Several partners have excellent records in recruiting and promoting female researchers. At HU Claudia Draxl and Sakia Fischer At IKZ Jutta Schwarzkopf, and at HZB Catherine Dubourdieu serve as role models as professors and department heads. In the initial recruitment round, 28% of hired PhD students and 13% of hired Postdocs were women- above the fields average. The same holds for the Board of Directors and the principal investigators. We recognize that further improvement is needed in future..

| Group | female | Male | % female |
|---|---|---|---|
| Scientific Advisory Bord | 1 | 4 | 17 |
| Board of Directors | 2 | 5 | 29 |
| Principal Investigators | 6 | 21 | 22 |
| Postdocs | 1 | 7 | 13 |
| PhD students | 5 | 13 | 28 |

All partners document A family-friendly working environment and human resources policies HUB, TUB, PDI, and IKZ are certified by "beruf und familie" GmbH; FBH and FHI hold "TOTAL E-QUALITY" certification. (continuous since 2009). with FBH additionally receiving the sustainability award. FHI also adheres to Max-Planck-Gesellschaft (MPG) principles on equal opportunities. Within GraFOx, female students receive internal mentoring from female PIs.. Career mentoring for female PhD students and postdocs is offered through TUBs proMotion program and the ProFiL program at HUB and TUB. Practical support for PhD students with children is being offered from HUB. Until end of year 3, the coordinator of GraFOx, Ms. Kai Hablizel, also served as Equal Opportunity Officer at PDI and supported when questions on equal opportunity arose.
GraFOx has also strong international profile: 60% of its scientists came from 17 countries across 4 continents. We successfully acquired international joint projects. Among them are two German Korean projects between IKZ and Seoul-National University (SNU) as well as PDI and SNU, and a German-French project involving PDI and CNRS. In addition, we secured photoelectron spectroscopy beamtime at Paul-Scherrer Insititut (Switzerland), and magnet time at Los Alamos National lab, USA.

## 5. Structures and collaboration

Structure of existing and new collaborations. The collaboration in GraFOx follows a clear workflow. The most basic mode is providing samples grown in cluster G "Growth" for subsequent analysis in the clusters P "Physical properties" or for device fabrication and testing in cluster D "Devices". Within cluster G collaboration is driven in particular by bulk oxide samples from project G1X, which serve as a substrate for thin film growth in projects G3P—G13. Close links between ab-initio theory and experimental efforts on crystal growth and physical properties have yielded multiple publications and ongoing joint studies. As a result, most GraFOx partners and associate partners collaborated across projects. Focused research topics have proven especially effective in fostering collaboration and support scientific exchange among partners, PhD candidates and postdocs across different clusters and projects. Most third-party funded projects are inherently collaborative (see P9/G13, P10/P11/G10/G11/G12, D1/D1G1/D1G2/D1P).
Table 5.1 summarizes collaborations among GraFOx full partners. In Table 5.2, the first four lines list our associate partners; the following five lines list our scientific advisory board; the remaining lines detail international collaborators outside GraFOx who contribute samples as well as experimental and theoretical capabilities that complement our own.
Newly established collaborations – both within GraFOx and with external institutions - are marked accordingly in Tables 5.1 and 5.2.

### Additional agreements

In 2021, the Paul-Drude-Institut für Festkörperelektronik has signed a memorandum of understanding (see Mou_Parma_2021.pdf) on international collaboration with the University of Parma, Italy. Based on it, a strong collaboration has been established on kappa and beta-$Ga_2O_3$ and PDI to host guest PhD students under co-advisership of Dr. Piero Mazzolini (former GraFOx postdoc) from the group of Prof. Roberto Fornari.
In December 2021, the Alexander von Humboldt Foundation honoured the collaboration of Prof. Kookrin Char, with the Leibniz-Institut für Kristallzüchtung GraFOx in the field of oxide semiconductors by a prestigious Humboldt Research Award. This award enables Prof. Kookrin Char to stay another year at the Leibniz-Institut für Kristallzüchtung.

Prof. Darell Schlom is appointed Leibniz Chair, which reflects a particularly close connection with IKZ in the field of strain engineering of Oxides and IKZ awarded an international fellowship to Prof. Nini Pryds.

Change of governance. The Fritz-Haber-Institute of the Max-Planck Society withdraw from the GraFOx II cooperation agreement in June 2021 (see GraFOxII_withdrawal_Fritz-Haber-Institut.pdf). In July 2021, Prof. Roman Engel-Herbert became director of the Paul-Drude-Institut and co-speaker of GraFOx. Dr. Klaus Irmscher, PI of project D1P retired in 2021. His designated successor is Dr. Andreas Fiedler, former PhD student of GraFOx. Projects G9D and G10 were discontinued in the second half of 2021 since the PI, Prof. Holger Eisele, left our associate partner Technical University Berlin.

## 6. Quality assurance

Quality control of the project is assured through measures established in GraFOx I. Overall progress of the project against objectives is monitored by the PIs and in monthly meetings with the PhDs and Postdocs. The project is overseen by a Scientific Advisory Board (SAB) of international pioneers in oxide electronics whose expertise spans GraFOx ´s interdisciplinary research areas. Excellence in recruitment is essential for project success. Open positions were advertised across the network and internationally; shortlisted candidates are interviewed by the responsible PIs. Each PhD signs a career development and research plan with their home institution. This plan is reviewed annually. Co-supervision (dual advisorship) is standard practice. Scientific outputs are submitted to peer-reviewed journals. At IKZ, FBH, FHI and PDI manuscripts also undergo internal review. Presentations for international conferences are rehearsed within the research groups and with GraFOx members prior to delivery.

## 7. Additional resources

According to our submitted **proposal for GraFOx II,** the **total co-funding** *in cash* and *in-kind* was **€5,435,330.00**. After positive grant notification, and communication of the Leibniz budget reduction by 25%, four GraFOx II full partner (IKZ, FBH, FHI and HZB) agreed to contribute €64,000 (€16,000 each) to compensate for the elimination of the Speakers budget (budget for network activities). However, due to FHI's withdrawal, they only contributed €91,780 (of which €54,280 *in-cash* and €37,500 *in-kind*) in 2020, a total of €424,220 less than intended. This **resulted** in **total co-funding** of **€5,069,177.74.** A total of € 5,190,533.06 co-funding (*in-cash, in-kind,* total personnel and other costs, e.g. travel) has been provided through the entire reporting period as detailed below.

| | in-kind | in-cash | total co-financing |
|---|---|---|---|
| Personnel | € 2,344,545.49 | € 1,815,946.37 | € 4,160,491.86 |
| Consumable | € 396,409.00 | € 633,632.20 | € 1,030,041.20 |
| total | € 2,740,954.49 | € 2,449,578.57 | € 5,190,533.06 |

## 8. Outlook

While application for a continuation of the network in a large-scale scientific network “Materials by Design” (Einstein Zentrum) funded by the Einstein foundation is currently pending, a number of individual and network projects have been and are being applied for at national and EU level by different GraFOx partners and their national and international collaborators.

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