

Part IV.

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Boards, directors, Max Planck fellows, and external scientific members

Supervisory board (as of June 2022)*

Prof. Dr. rer. nat. Klaus BLAUM (Chairman)**
Vice-president CPTS, Max-Planck-Society, Munich, Germany

Hans Jürgen KERKHOFF (Vice-Chairman)**
Steel Institute VDEh, Düsseldorf, Germany

Carl DE MARÉ**
ArcelorMittal Belgium N.V., Gent, Belgium

Dr.-Ing. h.c. Hans FISCHER**
Tata Steel Europe Ltd., Ijmuiden, the Netherlands

State Secretary Dr. Dirk GÜNEWIG**
Ministry of Culture and Science of the State of North Rhine-Westphalia, Düsseldorf, Germany

Univ.-Prof. Dr. rer. nat. Ulrich RÜDIGER
Rector, RWTH University Aachen, Germany

Prof. Dr. Martin PAUL
Rector, Ruhr-Universität Bochum (RUB), Bochum, Germany

Wolfgang SCHÜTZ
AG der Dillinger Hüttenwerke, Dillingen/Saar, Germany

* The supervisory board met for its last meeting in June 2022. The board was dissolved in the subsequent change to the shareholder structure of the institute and the associated amendments to the Articles of Association.

** This person is no longer active in the former function and/or company.

Scientific advisory board (as of April 2024)

Prof. Dr. Mark ASTA
University of California Berkeley, Berkeley, USA

Prof. Dr. Julie CAIRNEY
The University of Sydney, Sydney Camperdown, Australia

Prof. Dr. Fionn DUNNE
Imperial College London, London, UK

Prof. Dr. Lindsay GREER
University of Cambridge, Cambridge, UK

Prof. Dr. Eva OLSSON
Chalmers University of Technology, Göteborg, Sweden

Prof. Dr. George PHARR
Texas A&M University, College Station, USA

Prof. Dr. Mary P. RYAN
Imperial College London, London, UK

PD Dr. André SCHNEIDER
Thermo-Calc Software AB, Solna, Sweden

Prof. Dr. Christopher A. SCHUH
Northwestern University, Evanston, USA

Prof. Dr. Sannakaisa VIRTANEN
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany

Prof. Dr. Kerstin VOLZ
Philipps-Universität Marburg, Marburg, Germany

Prof. Dr. Bilge YILDIZ
Massachusetts Institute of Technology, Cambridge, USA

Directors, Max Planck fellows, and external scientific members

Directors:

Prof. Dr. rer. nat. Gerhard DEHM, (since Oct. 2012)

Prof. Dr. rer. nat. Jörg NEUGEBAUER (since Nov. 2004)*

Prof. Dr.-Ing. Dierk RAABE (since July 1999)**

* Provisional Head of the Department Interface Chemistry and Surface Engineering

** Chief Executive since 29th Sept. 2010 (re-elected 2015 and 2020)

Emeritus:

Prof. Dr. rer. nat. Martin STRATMANN (2000 - 2023 director, 2014 - 2023 on leave for the time of his presidency of the MPG, emeritus at the institute since June 2023)

Max Planck fellow:

Prof. Dr. Kristina TSCHULIK, Ruhr-Universität Bochum (since Sept. 2021)

External scientific members:

Prof. Dr. Mats HILLERT, Stockholm, Sweden (deceased Nov. 2022)

Prof. Dr. Reiner KIRCHHEIM, Göttingen

Guest scientists

Between January 2022 and August 2024, the Max Planck Institute for Sustainable Materials hosted in total **169** international guest scientists.

Alexander von Humboldt Foundation

29 of our guests joined us with awards and fellowships from the Alexander von Humboldt Foundation.

- **24** Humboldt Research Fellowships for Postdoctoral Researchers
- **2** Capes-Humboldt Research Fellowships for Postdoctoral Researchers
- **1** Humboldt Research Fellowship for Experienced Researchers
- **1** Humboldt Research Award for outstanding academic record
- **1** Friedrich Wilhelm Bessel Research Award

In November 2021, B. Gault and D. Raabe became **Humboldt scouts in the Henriette Herz Scouting Programme**. Each scout has the opportunity to recommend three research talents from abroad for a Humboldt Research Fellowship. After formal approval, the fellowships are granted directly. During the period of this report, three scientists have received a scholarship via the Henriette Herz Scouting Programme.

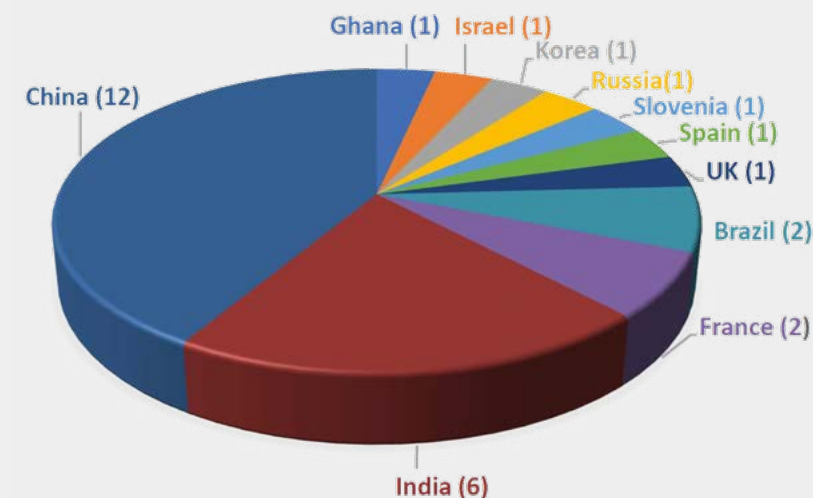
In the ranking of the Humboldt Foundation, the institute **was ranked first in Engineering Sciences** in 2023. It was also **ranked second place over all sciences** of non-university research institutions. The ranking covers the period 2018 – 2022.

Engineering Sciences

Universities		Other institutions		
Engineering Sciences				
↓ Absolute rankings	① Institution	Number of fellows	Number of award winners	↓ Total number
1	MPI für Eisenforschung (MPIE), Düsseldorf	36	3	39
2	MPI für Intelligente Systeme, Stuttgart und Tübingen	26	5	31
3	Helmholtz-Zentrum hereon, Geesthacht	11	1	12

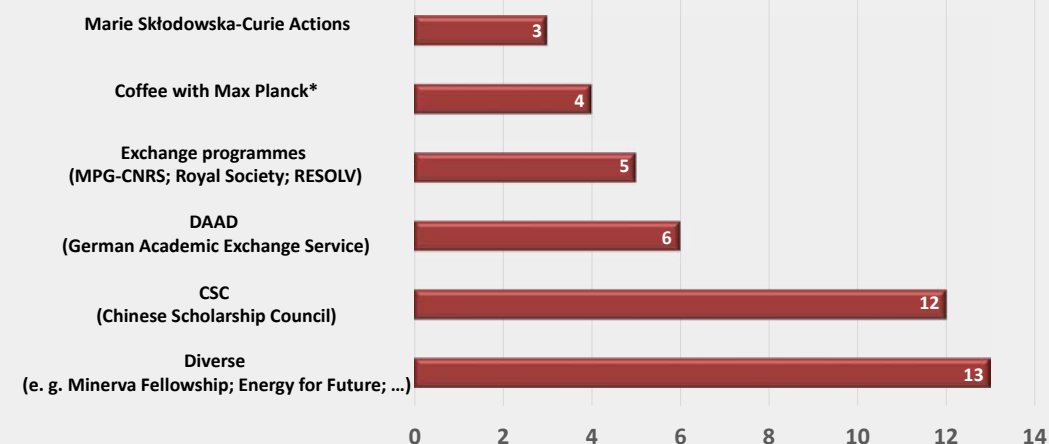
Source: <https://www.humboldt-foundation.de/en/explore/figures-and-statistics/humboldt-rankings#c18797>

Home countries of guests from the Alexander von Humboldt Foundation



Diverse fellowships

43 scientists came to the MPI-SusMat with other fellowships:

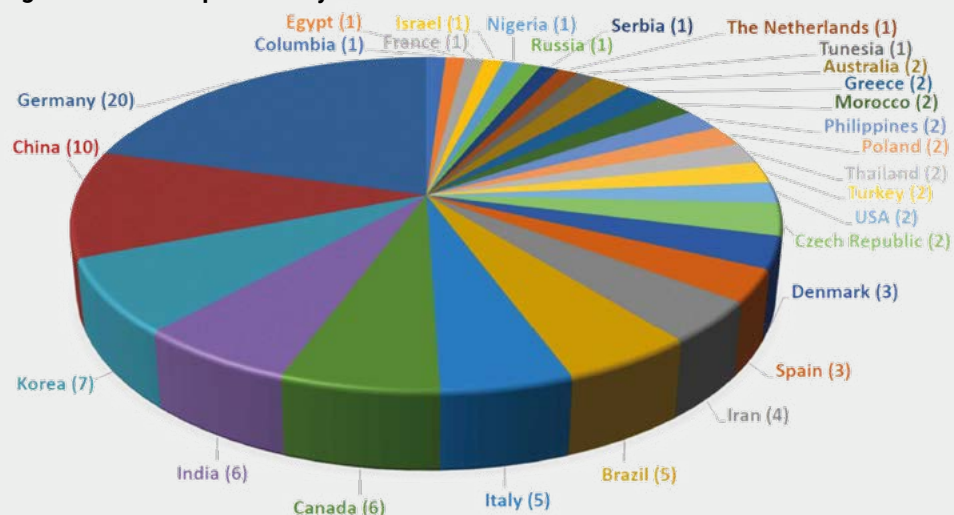


*Coffee with Max Planck: Seminar series which aims at recruiting talented young researchers to the institute (funded by the German Federal Ministry of Education and Research).

International research cooperation

Of **97** guest scientists, the majority stayed with us as part of research cooperations, **23** of them being MPI-SusMat alumni.

Number of guest scientists per country



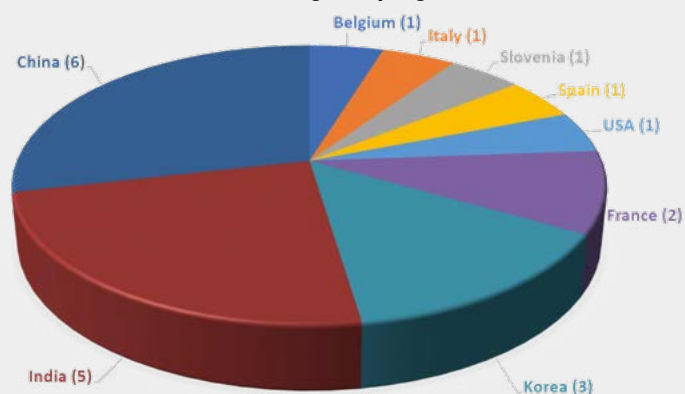
A detailed list of our "National and International Cooperation Partners" can be found from page 256 onwards.

MPI-SusMat guest programme

Our institute offers a postdoctoral guest programme for outstanding international scientists. The postdoc guests have the opportunity to introduce their research topic and exchange ideas with excellent colleagues, thus establishing important scientific networks for the future.

From January 2022 to August 2024 a total of **21** postdoctoral researchers from all over the world joined this guest programme, spending between 12 and 24 months at our institute.

Home countries of postdocs in the MPI-SusMat guest programme



Scientific honours & appointments

Honours

2022

B. Bellón: Acta Student Award 2022

B. Distl, F. Stein: Editor's Choice Award of Journal of Phase Equilibria and Diffusion

A. Garzón Manjon: Ramón y Cajal research grant from The Spanish Ministry of Economy and Competitiveness

F. Körmann: 2021 Editor's Choice article by the Editor-in-Chief of Journal of Phase Equilibria and Diffusion

A. Kwiatowski da Silva: Aaronson Award for outstanding contributions to the physical metallurgy of phase transformations, International Conference on Solid-Solid Phase Transformations in Inorganic Materials (PTM)

Y. Ma: DGM Young Talent Prize

Y. Ma: Member of Associate Editorial Board at the Materials Research Letters

D. Raabe: Acta Materialia Gold Medal

D. Raabe: Honorary Doctor at Norwegian University of Science and Technology

I. Souza Filho: The June 2022 Cover Paper of Journal of Materials Science

S. Yoo: One of 5 finalists for the Gerhard Ertl Young Investigator Award

H. Zhao: DGM Masing Memorial Prize

2023

J. P. Best: Georg-Sachs Prize 2023

B. Distl: Otto Hahn Medal of the Max Planck Society

C. Freysoldt: J. H. Block Lecture at the Atom Probe Tomography and Microscopy Conference 2023 in Leuven, Belgium

D. Lee: Winner of the Max Planck POSTECH/Korea Research Initiative for the 2023 Korea-Germany Junior Research Fellowship Program

C. Liu: Member of Youth Editorial Board, Acta Metallurgica Sinica

MPI-SusMat: 1st place in the Alexander von Humboldt Ranking in Engineering Sciences among all non-university research institutions & 2nd place overall sciences of non-university research institutions

D. Raabe: Van Horn Distinguished Lecturer

D. Raabe: NIMS Award 2023

M. Rohwerder: European Corrosion Medal 2023

T. Schwarz: E. W. Müller Outstanding Emerging Scientist Award

M. Stratmann: Member of the HGI Board of Trustees, Horst-Görtz-Institut (HGI), Bochum, Germany

M. Todorova: Alexander Kuznetsov Prize for Theoretical Electrochemistry

2024

E. Bitzek: Elected to the Review Board of the German Research Foundation (DFG)

J. Neugebauer: 2024 ISMM Distinguished Career Award, International Society on Materials Modeling (ISMM)

T. Schwarz: Walter Benjamin Grant, German Research Foundation (DFG)

P. Sokolinski: European Placement Prize of Cambridge University

M. Stratmann: Chairman of the International Advisory Board of the UA Ruhr, University Alliance Ruhr, Germany

M. Stratmann: Member of the Board of Trustees of the kata agorein Foundation, kata agorein Stiftung, Bamberg, Germany

M. Vega Paredes: Selected as Young Scientist Participant – 73rd Lindau Nobel Laureate Meeting Physics (Lindau, Germany)

Career programmes for female scientists

N. Cheng: Selected to participate in the MPG Sign Up! For Leadership in 2022

A. Kanjilal: Selected to participate in the MPG Sign Up! Career Development in 2022

A. Saksena: Selected to participate in the MPG Sign Up! Career Development in 2023

D. Smirnova: Selected to participate in the MPG Sign Up! For Leadership in 2023

D. Sonawane: Selected to participate in the MPG Sign Up! Career Development in 2022

M. Todorova: Boost! Programme of the MPG

J. Yang: Selected to participate in the MPG Sign Up! Career Development in 2022

MPI-SusMat trainees

2023

H. Bögershausen: Golden Badge of Honour for 20 years of service on the examination board, IHK (chamber of industry and commerce) Düsseldorf (Germany)

H. Faul: Golden Badge of Honour for 20 years of service on the examination board, IHK (chamber of industry and commerce) Düsseldorf (Germany)

S. Flaum: "Chambers best 2023" in the field of industrial mechanics, IHK (chamber of industry and commerce) Düsseldorf (Germany)

Z. Meshou: "Chambers best 2023" in the field of material testing, IHK (chamber of industry and commerce) Düsseldorf (Germany)

L. Monaghan: "Chambers best 2023" in the field of material testing, IHK (chamber of industry and commerce) Düsseldorf (Germany)

2024

S. Flaum: Max Planck Trainee Award 2024 of the Max Planck Society (Germany)

J. Kuschke: Max Planck Trainee Award 2024 of the Max Planck Society (Germany)

Paper, poster, excellence in reviewing, travel and communication awards

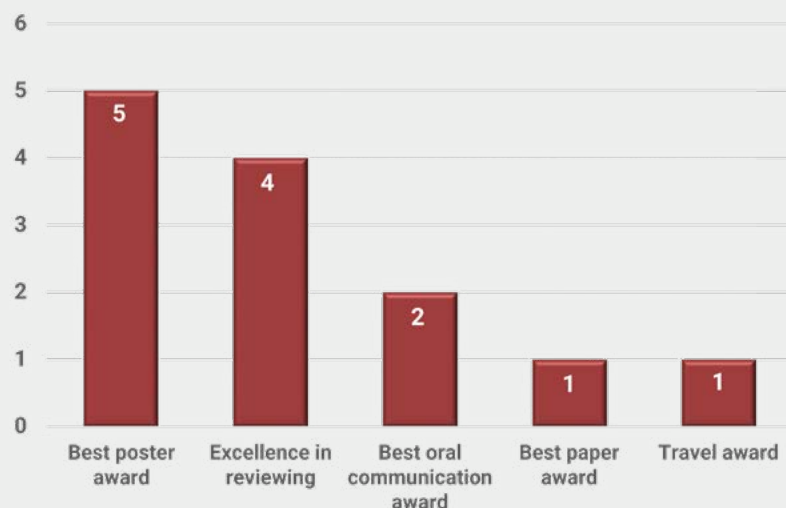
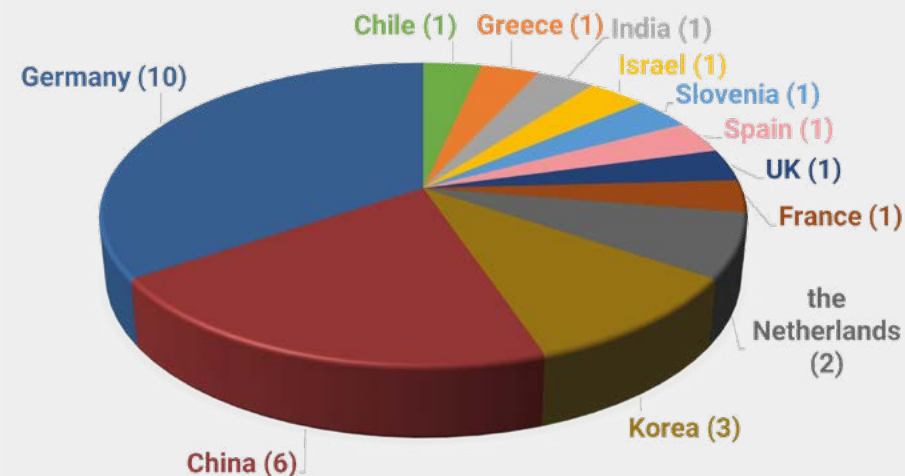


Fig.1: Summary of all best paper, best poster, excellence in reviewing, travel and communication awards received by MPI-SusMat scientists between 2022 – 2024. These awards are not listed above.

Appointments

Destination countries of appointments



2021 (not included in Scientific Report 2019-2021)

S. Antonov: Research Physical Scientist, National Energy Technology Laboratory, Albany, Oregon, United States

L. Belkacemi: Group leader for atom probe tomography laboratory, Leibniz-Institut für Werkstofforientierte Technologien – IWT, Bremen, Germany

C. Jung: Associate Professor, Pukyong National University, South Korea

G. Wu: Full Professor, Xi'an Jiao Tong University, China

W. Xia: Director at the Anhui University of Technology, Ma'anshan, Anhui, China

J. Zavašnik: Assistant Professor at the Jožef Stefan International Postgraduate School, Slovenia

2022

H. Bishara: Senior Lecturer, The Iby and Aladar Fleischman Faculty of Engineering, Tel Aviv University, Israel

C. Liu: Full Professor, Xi'an Jiao Tong University, China

L. Lymparakis: Associate Professor, Department of Physics, University of Crete, Greece

F. Roters: Associate Professor, Faculty of Georesources and Materials Engineering, RWTH Aachen, Germany

I. Souza Filho: Evaluator at the National Research and Development Agency (ANID) of the Ministry of Science, Technology, Knowledge and Innovation of Chile

S. Wippermann: Professorship for "Green Energy Materials", Department of Physics, Philipps-Universität Marburg, Germany

2023

K. Devi: Assistant Professor, Indian Institute of Technology, India

A. Garzón Manjón: Associate Professor, Department of Chemistry, Universitat Autònoma de Barcelona, Spain

S. G. Kang: Assistant Professor, Division of Materials Science and Engineering, Gyeongsang National University, South Korea

S.-H. Kim: Assistant Professor, Korea University, Seoul, South Korea

I. Souza Filho: Assistant Professor, Institut Jean Lamour, CNRS, Université de Lorraine, France

M. Stratmann: Group Leader of Emeritus Group of Electrochemical Surface Science, Independent Research Groups, Max Planck Institute for Sustainable Materials, Germany

D. Xie: Full Professor, Xi'an Jiao Tong University, China

H. Zhao: Full Professor, Xi'an Jiao Tong University, China

2024

Y. Bai: Assistant Professor, Great Bay University, China

R. Dubosq: Assistant Professor, University of British Columbia, Okanagan, Canada

C. Liebscher: Professor for Advanced Transmission Electron Microscopy at the Faculty for Physics and Astronomy at the Ruhr-Universität Bochum and the Research Center Future Energy Materials and Systems (RC FEMS), Germany

Y. Ma: Assistant Professor, Materials Science and Engineering, Delft University of Technology, The Netherlands

Z. Rao: Associate Professor at Shanghai Jiaotong University, China

H. Springer: Full Professor, Faculty of Georesources and Materials Engineering, RWTH Aachen, Germany

F. Worsnop: Lecturer, Department of Materials, Imperial College London, UK

Y. Wu: Lecturer, Department of Materials Science and Engineering, Monash University, Australia

Participation in research programmes 2022 – 2024

National

BMBF

HINT - Highspeed in situ nanomechanical tester

H₂Giga flagship:

- Prometh2eus - Project network for optimised material development for technical H₂ generation through improved oxygen electrodes

MaterialDigital - Joint project: Innovation platform
Material Digital - sub-project: Software tools

StahlDigital - Workflows and Platformintegration

White-Etching-Cracks - Knowledge-based design of wear-resistant bearing steels through characterisation at the atomic level A way out of the "white etching crack" problem of wind turbines

BMWK

HEPCO - Hydrogen Embrittlement Protection Coating

MODUL - Integrated material and process development of high-modulus steels

MODULUS - High modulus steels for the additive manufacturing of lightweight components

PAULL2 - Development of MEA for the Activation of Ultra-Long Lifetimes 2 (PAULL2), Subproject: Elucidation of the structure and stability of new catalysts and support materials by electron microscopy

S3-Alu - Simulation Methodologies for the Evaluation of Components and Systems for Sustainable Lightweight Construction with Secondary Aluminum; part project: mechanical phase properties and effective mechanical properties

DFG

DFG awards

Gottfried Wilhelm Leibniz Award 2020 for B. Gault

Walter Benjamin position for Y. Ma and T. Schwarz

DFG Collaborative Research Centres (SFB), trans-regio projects (TRR) & priority programmes (SPP)

SFB 1394: Structural and Chemical Atomic Complexity: From Defect Phase Diagrams to Material Properties

- A01: Solid solution effects on the formation of defect phases in Ni-X solid solutions
- A02: High-throughput simulations of dislocation and grain boundary defect phases
- B04: Passivating oxide phases in the Ni/X/H₂O System
- B06: Grain boundary phases in Ni, Ni-Cu and Ni-Au solid solution films
- B08: Formation of defect phases via hydrogen exposure in nickel alloys
- C01: Multiphysics Description of Metal-Intermetallic Composites at the Grain Scale (1st period until 2023)
- C05: Ab initio thermodynamics of defect phases
- T01n: From experimental and atomistic simulation data to Calphad assessments

SFB 1625: Atomic-scale understanding and design of multifunctional compositionally complex solid solution surfaces (1st Phase, 2024–2027)

- A02: Microstructure design of quasi-single-crystalline and smooth model thin films
- A04: Ab initio simulations of electrochemical reactions at CCSS surfaces
- B03: High resolution (scanning) transmission electron microscopy investigation of the surface and other defects in CCSS
- B04: Enabling (quasi)-in-situ analytical field-ion microscopy of active CCSS catalysts

TRR 103: From Atoms to Turbine Blades – A Scientific Approach for Developing the Next Generation of Single Crystal Superalloys (3rd Phase, 2020–2023)

- A04: Investigation of the local alloy composition by atom probe tomography
- C03: Atomistic simulations of elementary dislocation processes in coherent and semi-coherent γ/γ' -microstructures: influence of temperature and composition
- T13: Influence of H on phase stability and mechanical properties of single-crystal Ni-based superalloys (2024–2027)



TRR 188: Damage Controlled Forming Processes

- B03: Position resolved damage nucleation and growth at the microstructure length scale

TRR 270: Hysteresis design of magnetic materials for efficient energy conversion (1st Phase, 2020–2023, 2nd Phase, 2024–2027)

- Z01: Advanced analytical electron microscopy and atom probe tomography
- T02: Machine-learning for atom probe tomography (2024–2027)

SPP 2006: Compositionally Complex Alloys – High Entropy Alloys (CCA – HEA)

- MULTITRIPCCA-s – Design and mechanical properties of compositionally complex alloys from twinning-induced towards bidirectional transformation-induced plasticity

SPP 2370: Interlinking catalysts, mechanisms and reactor concepts for the conversion of dinitrogen by electrocatalytic, photocatalytic and photoelectrocatalytic methods (“Nitroconversion”)

- Photoelectrochemical Nitrogen Reduction: Activity, Selectivity and Stability of Cu-based Ternary Oxide Photocathodes

DFG research grants

Ab initio determination of free energies and derived properties (heat capacities, vacancies, solvus boundaries) for selected alloys containing Si, Mg and Cu

Correlative Scanning Precession Electron Diffraction and Atom Probe Tomography to access the 3D polycrystalline grain microstructure of nanomaterials

Elementary mechanisms of tribologically-induced oxidation in copper

Machine learning the thermodynamics of complex materials with ab initio accuracy

Multiscale investigation of impact mitigation strategies: Biomimicking musk ox head

Revealing the causes of the unusual mechanical behavior of B2 FeAl compounds

DFG Cluster of Excellence

EXC 2033: RESOLV (Ruhr Explores Solvation)

DFG International Cooperation

Atomic-level characterization of sulfide solid-electrolyte battery

DFG German-Israeli Project Cooperation

MXene-based energy materials guided by 3D Atomic-Resolution Tomography

DFG Walter Benjamin programme

Multiscale and operando studies on the role of micro- and nanostructures in the direct reduction of hydrogen-based iron oxides

Resolving the reactive liquid-solid corroding interface at the near atomic level to understand the influence of alloy and electrolyte composition (CorrInt)

DFG Research Training Groups

GRK 1896: In Situ Microscopy with Electrons, X-Rays and Scanning Probes

NFDI technical and methodological consortia

FAIRmat – FAIR Data Infrastructure for Condensed-Matter Physics and the Chemical Physics of Solids

NFDI-MatWerk - National Research Data Infrastructure for Materials Science & Engineering

Max Planck Society

IMPRS SusMet - International Max Planck Research School for Sustainable Metallurgy - from Fundamentals to Engineering Materials

MaxNet BiGmax - Max Planck Research Network on big-data-driven material science

Max Planck Africa Mobility Grant on High-performance Hard Carbon Anode Materials

Max Planck Fellow Group on Electrochemistry & Nanoscale Materials (Kristina Tschulik)

Max Planck partner groups

Max Planck partner group (India): Combinatorial design of novel high-performance permanent magnets

Max Planck partner group (India): Designing damage tolerant functional oxide nanostructures

Max Planck partner group (India): Environmental degradation of high-temperature materials in service conditions

Max Planck partner group (India): Stress and defects-driven phase transformations

Max Planck partner group (Israel): Physical properties of decorated grain boundaries: segregation and precipitation

Max Planck partner group (Korea): Electron beam irradiation-based deformation processes in 3D nano-architectured oxides

Max Planck partner group (Slovenia): Microstructure design of high-performance materials for harsh energy applications

Max Planck-Fraunhofer collaboration

MaRS - Critical materials lean Magnets by Recycling and Substitution

Helmholtz

Helmholtz Data School for Life, Earth, and Energy (HDS-LEE)

Ministry of Economic Affairs, Industry, Climate Protection and Energy of the State of North Rhine-Westphalia

progress.nrw

Coat4Hydrogen - Complex alloy coatings for steel of the highest corrosion resistance in hydrogen applications

KSB Stiftung

FeOx-HOTMECH - Nano- and micromechanics of iron ore model systems at high temperature: Toward designer feedstocks for CO₂-free hydrogen-based direct reduction

International

European Union

ERC (European Research Council)

AMMicro - Additive Micromanufacturing: Multimetal Multiphase Functional Architectures

GB-CORRELATE - Correlating the State and Properties of Grain Boundaries

microKlc - Microscopic Origins of Fracture Toughness

ROC - Reducing Iron Oxides without Carbon by using Hydrogen-Plasma

SHINE - Seeing hydrogen in matter

Marie Skłodowska-Curie Actions

CryoFusion - Improving surface and bulk properties of promising fusion material using deep cryogenic treatment

DyThM-FCC - Dynamic thermomechanical deformation map of FCC microparticles using additive micromanufacturing and machine learning

FP-RESOMUS - Fellowship Program of the NCCR MUST (National Competence Center for Research in Molecular Ultrafast Science and Technology) and the Cluster of Excellence RESOLV-FP-RESOMUS

MetaSCT - Metamaterials for Thermoelectric Applications - multiscale Structure, Chemistry, Thermal Property relations to uncover the local behavior of grain boundaries

REDI - Redi-RMIT European Doctoral Innovators Programme

Collaborative Projects

ADVANCE - Sophisticated experiments and optimisation to advance an existing CALPHAD database for next generation TiAl alloys

FORGE - Development of novel and cost-effective coatings for high-energy processing applications

HAIMan - Sustainable Hydrogen and Aluminothermic Reduction Process for Manganese, its alloys and Critical Raw Materials Production

H2Free - Investigation and modelling of hydrogen effusion in electrochemically plated ultra-high-strength-steels used for landing gear structures

H2PlasmaRed - Hydrogen Plasma Reduction for Steel-making and Circular Economy

HyWay – Multiscale Characterisation and Simulation for Hydrogen Embrittlement Assessment: Development of an Open Knowledge Platform to Foster Capability Integration

Nano-S-Mart - Unlocking the effect of residual elements via the Nanoengineering of Sustainable Martensitic steels

EIC (European Innovation Council)

CoCoMag - Multi-property Compositionally Complex Magnets for Advanced Energy Applications

Heat2Battery - All in One: Harvesting of waste heat with solid thermal battery

RFCS (Research Fund for Coal and Steel)

DELIGHTED - Design for Lightweight Steel for Industrial Applications

HYDRO-REAL - Hydrogen Interaction with Retained Austenite Under Static and Cyclic Loading Conditions

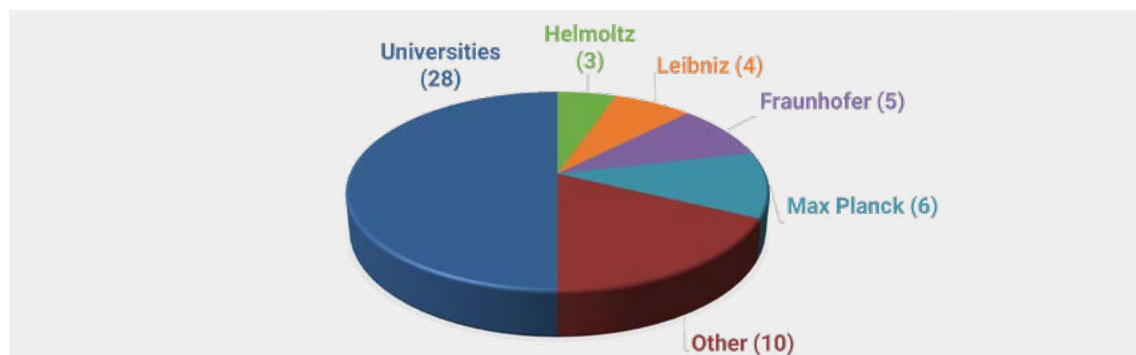
RVO (Rijksdienst voor Ondernemend Nederland)

Groeien met Groen Staal



Collaboration with national and international universities and research institutes

National



Universities

Bergische Universität Wuppertal	Technische Universität Darmstadt
Christian-Albrechts-Universität zu Kiel	Technische Universität Dortmund
Friedrich-Alexander-Universität Erlangen-Nürnberg	Technische Universität München
Heinrich-Heine-Universität Düsseldorf	Universität Bayreuth
Justus-Liebig-Universität Gießen	Universität Bielefeld
Karlsruher Institut für Technologie – KIT	Universität Bremen
Ludwig-Maximilians-Universität München	Universität der Bundeswehr München
Otto-von-Guericke-Universität Magdeburg	Universität Duisburg-Essen
Philipps Universität Marburg	Universität Freiburg
Ruhr-Universität Bochum	Universität Konstanz
RWTH Aachen	Universität Münster
Technische Universität Bergakademie Freiberg	Universität Paderborn
Technische Universität Berlin	Universität Siegen
Technische Universität Clausthal	Universität Stuttgart

Research institutes

ACCESS e.V.	Forschungszentrum Jülich GmbH
Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin	Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V.
Deutsche Akademie der Naturforscher Leopoldina, Halle	Fraunhofer-Institut für Lasertechnik (ILT), Aachen
Deutsches Zentrum für Luft- und Raumfahrt (DLR), Bonn	Fraunhofer-Institut für Umwelt- Sicherheits- und Energietechnik UMSICHT, Oberhausen
fem Forschungsinstitut für Edelmetalle und Metallchemie, Schwäbisch Gmünd	Fraunhofer-Institut für Werkstoffmechanik (IWM), Freiburg

Fraunhofer-Institut für Werkstoff- und Strahltechnik (IWS), Dresden

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Helmholtz-Institut Erlangen-Nürnberg (HI ERN) für Erneuerbare Energien, Erlangen

Helmholtz-Zentrum Berlin (HZB) für Materialien und Energie, Berlin

Helmholtz-Zentrum hereon GmbH: Institut für Werkstoffphysik, Geesthacht

Institut für Angewandte Informatik e.V. (InfAI), Leipzig

Institut für Umwelt & Energie, Technik & Analytik e.V. (IUTA), Duisburg

Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW), Dresden

Leibniz-Institut für Neue Materialien (INM), Saarbrücken

Leibniz-Institut für Plasmaforschung und Technologie e.V. (INP), Greifswald

Leibniz-Institut für Werkstofforientierte Technologien (IWT), Bremen

Max-Planck-Institut für Chemische Energiekonversion, Mülheim an der Ruhr

Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr

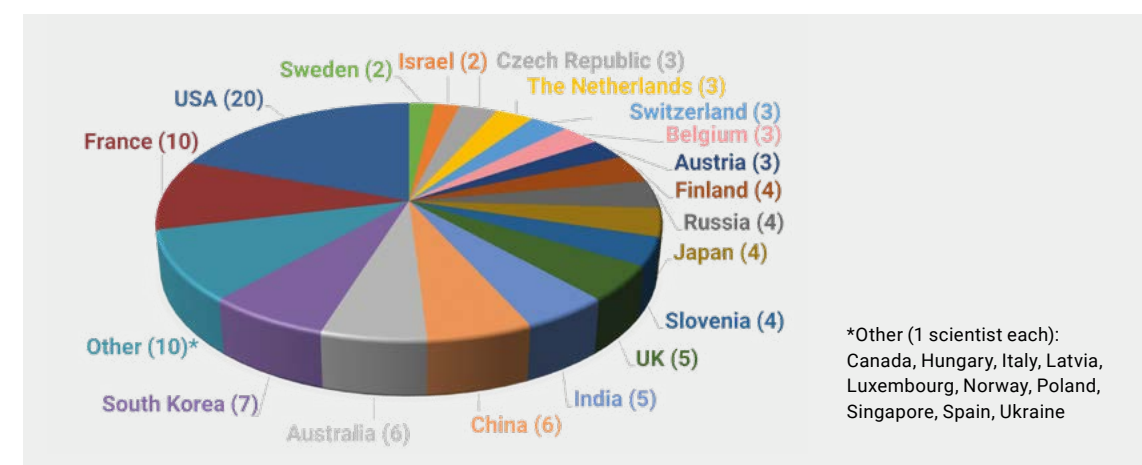
Max-Planck-Institut für Festkörperforschung, Stuttgart

Max-Planck-Institut für Intelligente Systeme, Stuttgart

VDEh-Betriebsforschungsinstitut GmbH (BFI), Düsseldorf

Zentrum für Brennstoffzellen-Technik GmbH (ZBT), Duisburg

International



*Other (1 scientist each):
Canada, Hungary, Italy, Latvia,
Luxembourg, Norway, Poland,
Singapore, Spain, Ukraine

Universities

Aalto University, Finland	Switzerland
Aix-Marseille University, France	Guangxi University, Nanning, China
Belgorod State University, Russia	Gyeongsang National University, Seoul, South Korea
Brown University, Providence, Rhode Island, USA	Hasselt University, Belgium
Central South University, Changsha, China	Hokkaido University of Science, Sapporo, Japan
Charles University, Prague, Czech Republic	Imperial College London, UK
Clemson University, South Carolina, USA	Indian Institute of Technology Bombay, India
Cranfield University, England, UK	Indian Institute of Technology Chennai, India
Delft University of Technology, The Netherlands	Indian Institute of Technology Madras, India
École Polytechnique Fédérale de Lausanne (EPFL),	Indian Institute of Technology Roorkee, India



Kangwon National University, Chuncheon, South Korea
Katholieke Universiteit Leuven, Belgium
Korea University, Seoul, South Korea
KTH Royal Institute of Technology, Stockholm, Sweden
Kurdyumov Institute of Metal Physics, Ukraine
Leiden University, The Netherlands
Linköping University, Sweden
Luxembourg Institute of Science and Technology (LIST), Luxembourg
Massachusetts Institute of Technology (MIT), Cambridge, Massachusetts, USA
MINES ParisTech PSL Research University, France
Monash University, Melbourne, Australia
Montanuniversität Leoben, Austria
National University of Science and Technology (MISiS), Moscow, Russia
North Carolina State University, Raleigh, North Carolina, USA
Northwestern University, Illinois, USA
Norwegian University of Science and Technology (NTNU), Trondheim, Norway
Riga Technical University, Latvia
RMIT Europe, Spain
Royal Melbourne Institute of Technology (RMIT), Australia
Silesian University of Technology, Gliwice, Poland
Singapore University of Technology and Design (SUTD), Singapore
Southern University of Science and Technology, Shenzhen, China
Tampere University, Finland
Technical University Eindhoven, The Netherlands

Technical University of Liberec, Czech Republic
Tel Aviv University, Tel Aviv, Israel
Texas A&M University, College Station, TX, USA
Tongji University, Shanghai, China
Université Paris-Est Créteil, ICMPE, Thiais, France
Université Paris-Saclay, CEA, Gif-Sur-Yvette, France
Université Sorbonne Paris Nord, France
University of British Columbia Vancouver, Canada
University of California, Berkeley, California, USA
University of California, Santa Barbara, California, USA
University of California, Los Angeles, California, USA
University of Cambridge, UK
University of Chicago, IL, USA
University of Connecticut, USA
University of Florida, Gainesville, USA
University of Helsinki, Finland
University of Illinois, Urbana-Champaign, USA
University of Manchester, UK
University of New South Wales, Australia
University of Oxford, UK
University of Queensland, Brisbane, Australia
University of Sydney, Australia
University of Texas, Austin, TX, USA
University of Ulsan, South Korea
University of Vienna, Austria
University of West Bohemia, Pilsen, Czech Republic
Vrije Universiteit Brussel, Belgium
Xi'an Jiaotong University, Xi'an, Shaanxi, China

Research institutes

Argonne National Laboratory, Lemont, IL, USA
ARMINES – Association pour la recherche et le développement des méthodes et processus industriels, France
Austrian Academy of Sciences, Leoben, Austria
Australian Nuclear Science and Technology Organisation (ANSTO), Australia
Budapest Neutron Centre (BNC), Hungary
CEA Paris-Saclay, France

Centre de Mise en Forme des Matériaux (CEMEF), Nice, France
Centre National de la Recherche Scientifique (CNRS): Centre Interdisciplinaire de Nanoscience de Marseille (CiNAM), Luminy, Marseille, France
Centre National de la Recherche Scientifique (CNRS): Office National d'Etudes et de Recherches Aérospatiales (ONERA), Châtillon, France
Center of Excellence on Nanoscience and Nanotechnology (CENN Nanocenter), Slovenia

Council of Scientific and Industrial Research, National Metallurgical Laboratory (CSIR-NML), Bhubaneswar, India

Czech Academy of Sciences, Brno, Czech Republic
Elettra Sincrotrone Trieste, Italy

Empa – Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland

Institut de Physique et Chimie de Matériaux de Strasbourg, France

Institute of Metals and Technology (IMT), Ljubljana, Slovenia

Institute of Quantum Materials Science, Yekaterinburg, Russia

Jožef Stefan Institute, Slovenia

Kangwon National University, Chuncheon, South Korea

Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea

Korea Institute of Industrial Technology (KITECH), Busan, South Korea

Lawrence Berkeley National Laboratory: Molecular Foundry, National Center for Electron Microscopy, Berkeley, USA

Lawrence Livermore National Laboratory, Livermore, CA, USA

Los Alamos National Laboratory, New Mexico, USA

National Institute of Chemistry, Ljubljana, Slovenia

National Institute for Materials Science (NIMS), Tsukuba, Japan

National Institute of Advanced Industrial Science and Technology (AIST), Tokyo, Japan

Paul Scherrer Institut (PSI), Switzerland

Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

Skolkovo Institute of Science and Technology, Moscow, Russia

Technion – Israel Institute of Technology, Haifa, Israel

Tokyo Institute of Technology, Japan

VTT Technical Research Centre of Finland, Finland





Collaborating industrial partners and patents

National

AG der Dillinger Hüttenwerke	NTTF Coatings GmbH
Altana AG	Otto Junker GmbH
BMW Group AG	Outokumpu Nirosta GmbH
Deloro Wear Solutions GmbH	point electronic GmbH
De Nora Deutschland GmbH	Robert Bosch GmbH
Dr. Wolfgang Kochanek Entwicklungsgesellschaft	Rolls-Royce Deutschland Ltd & Co KG
Freudenberg e-Power Systems GmbH	Salzgitter Mannesmann Forschung GmbH
Graebener Maschinentechnik GmbH & Co. KG	Schott AG
Heraeus Holding GmbH	Siemens AG
Infineon Technologies AG	Speira GmbH, Research & Development
inpro – Innovationsgesellschaft für fortgeschrittene Produktionssysteme in der Fahrzeugindustrie mbH	thyssenkrupp Steel Europe GmbH
kiutra GmbH	thyssenkrupp Uhde GmbH
KSB Stiftung	Umicore AG & Co. KG
Leistritz Turbinentechnik GmbH	VDM Metals International GmbH, Research & Development
Materials Science International Services GmbH (MSI)	Volkswagen AG
MTU Aero Engines AG	

International

AMAG Austria Metall AG, Austria	Materials Center Leoben Forschung GmbH, Austria
Alemnis AG, Switzerland	Nardi Compressori, Italy
Aperam Stainless Precision, France	OCAS NV (OnderzoeksCentrum voor de Aanwending van Staal), Belgium
Cambridge Nanolitic Limited, England, United Kingdom	Rolls-Royce Motor Cars Ltd., England, United Kingdom
c-sense GmbH, Austria	RTD Talos Ltd., Cyprus
Denso Corporation, Japan	Sandvik Coromant R&D, Sweden
ELHCO – Electroless Hard Coat S.A., Spain	Senai FIEMG, Brazil
Elsyca NV, Belgium	SIA DATI Group, Latvia
Exaddon AG, Switzerland	Sidenor Aceros Especiales, S.L., Spain
Fundación Azterlan, Spain	The Quartz Corp, Norway
Fundación Cidetec, Spain	Tata Steel Europe Ltd., The Netherlands
Infineon Technologies Austria AG, Austria	Tescan XRE, Belgium
JFE Steel Corporation, Japan	Thermo-Calc Software AB, Sweden
KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH, Austria	Vallourec Research Center France, France
Kobe Steel Ltd., Japan	Wärtsilä Finland Oy, Finland
	WinGD – Winterthur Gas & Diesel Ltd., Switzerland



Patents

Patents issued in the given time schedule

Date of Issue	Description	Inventors
September 18, 2023	DAMASK - the Düsseldorf advanced material simulation kit– word trademark (Wortmarke) (AZ 30 2023 115 397.4)	Roters, F. Eisenlohr, P. Diehl, M. Shantraj, P. Reuber, C.
December 12, 2022	Temperature Measurement for a High Temperature Micro-deformation Device (EP 18199374.2 & DE 602018044438.6)	Arigela, Viswanath Gowtham Kirchlechner, Christoph Gonzalez, Ivan Kölling, Michael
October 17, 2022	Process for manufacturing of microarchitectures (EP22201973.9. & PCT/EP2023/078833)	Ramachandramoorthy, R. Sung-Gyu, K.

Patents - overview

Date of issue	Description	Inventors
June 05, 2015 - 2023	Korrosionsbeständiger TWIP-Stahl (JP 2011-553279)	Weber, Sebastian Mujica Roncery, Lais
utility patent from August 18, 2016, prolonged August 31, 2019 until August 2022	Multi purpose method cell (20 2016 104 543.6)	Kerger, Philip Rohwerder, Michael
January 28, 2020 June 9, 2021	Process for recycling of noble metals (DE 102015118279.3, PCT/ DE2016/ 100498, EP 3 368 698 & USA 15/771,500)	Mayrhofer, Karl Hodnik, Nejc Baldizzone, Claudio
June 07, 2018	Fabrication of nanoporous carbide membranes Joint invention with Universitat Politècnica de Catalunya (EP 2 664 683 & (DE) 60 2012 047 997.3)	Renner, Frank Duarte-Correa, Maria Jazmin Lengsfeld, Julia Bruna, Pere, Barcelona Tech
March 03, 2016	Nanoelektroden-Partikelfalle für empfindliche spektroskopische und elektronische Analyse Joint invention with Academia Sinica Taipei, who is applicant (TWI490487 & US-Patent: Appl. No. 13/872,013 US 2014/0320849A2)	Erbe, Andreas Chia-Fu Chu Ming-Li Chu Leonardo Lesser-Rojas, all Academia Sinica, Taipei
January 8, 2015	Schichtsystem zum Korrosionsschutz ASKORR Joint invention with MPI für Polymerforschung and Fraunhofer Gesellschaft (DE 10 2012 209 761.9)	Rohwerder, Michael Vimalanandan, Ashokanand Tran, The Hai Landfester, K. Crespy, D. Fickert, J., MPI für Polymerforschung

Conferences, symposia and meetings organized by the institute

2021 (not included in the Scientific Report 2019 - 2021)

M. Rabe co-organized the "RESOLV 1st Online Summer School Solvation Science", held online, 25 - 26 May 2021

2022

G. Dehm, C. Scheu, R. Ramachandramoorthy and D. Sonawane organized the Symposium "Mechanics Meets Energy 2022" at Ringberg Castle, Bavaria (Germany), 10 - 14 Jan 2022

F. Stein and M. Palm co-organized the "6th MSIT Winter School on Materials Chemistry", held online, 03 - 07 Apr 2022

G. Dehm, G. Weikum (MPICS) and J. Neugebauer organized the "BiGmax Workshop 2022 on Big-Data-Driven Materials Science" at the University Conference Centre, Bochum (Germany), 11 - 13 Apr 2022

M. Todorova and C. Freysoldt organized the "Electrified solid/water interfaces – theory meets experiment Workshop" at Ringberg Castle, Bavaria (Germany), 15 - 18 May 2022

M.J. Duarte, A. Lassnig and B.-S. Li organized the Symposium "Mechanical Properties and Adhesion" at the 48th International Conference on Metallurgical Coatings & Thin Films (ICMCTF 2024), San Diego, CA (USA), 22 - 27 May 2022

M. Rabe co-organized the "RESOLV 8th Summer School on Solvation Science" at ZEMOS, Bochum (Germany), 07 - 10 Jun 2022

L. Gomell and B. Gault, organised the 8th NRW – Atom Probe Tomography user meeting (online) 08 June 2022

J. Neugebauer, O. Hegde, S. Menon, M. Poul, S. Surendralal, J. Behler, A. Bochkarev, R. Drautz, T. Hammer-schmidt, M. Herbold, C. Hermichen, A. Knoll, A. Kraych, N. Leimeroth, V. Lenz, Y. Lysogorskiy, L. Merl, M. Mrovec, M. Qamar, J. Rohrer, M. Schäfer and D. Voicu organized the "Potentials: From Electrons to Phase Diagrams Workshop" at the Ruhr-University-Bochum, Bochum (Germany), 08 - 10 Jun 2022

G. Dehm organized the Mini-Symposium "Experimental Micromechanics and Nanomechanics" at the 11th European Solid Mechanics Conference (ESMC 2022), Galway (Ireland), 04 - 08 July 2022

J. Neugebauer, K. Kremer and M. Scheffler organized the Symposium "SYNM: From Physics and Big Data to the Design of Novel Materials" at the DPG Spring Meeting 2022, Regensburg (Germany), 04 - 09 Sep 2022

Y. Ma and I. Souza Filho organized the "International Workshop on Sustainable Metallurgy of Green Steel (GreenSteel2022)", held online, 12 - 13 Sep 2022

M. Rohwerder organized the Symposium "C04 - Electrochemical Techniques in Corrosion Research" at the 242nd ECS Meeting, Atlanta (USA), 9 Oct 2022

K. Albe, J. Behler, R. Drautz, M. Mrovec, J. Neugebauer, J. Rohrer, A. Stukowski and Y. Lysogorskiy organized the Hands-on Workshop "Construction and Deconstruction of interatomic Potentials" at Reissensburg Castle, Günzburg, Bavaria (Germany), 18 - 22 Oct 2022

F. Stein and M. Palm co-organized the 1st "MSIT Advanced School on Diffusion in Materials - Fundamentals and Applications" at Ebernburg Castle, Rheinland-Pfalz (Germany), 24 - 26 Oct 2022

2023

G. Dehm, C. Scheu, L. Bhaskar and S. Pemma organized the Symposium "Mechanics Meets Energy 2023", Kloster Steinfeld, Kall (Germany), 29 Jan - 02 Feb 2023

G. Dehm organized the Symposium "Metals and Alloys" at the Microscopy Conference 2023, Darmstadt (Germany), 27 Feb - 02 Mar 2023

F. Stein and M. Palm co-organized the "7th MSIT Winter School on Materials Chemistry" at Ringberg Castle, Bavaria (Germany), 12 - 16 Mar 2023

E. Bitzek, R. Janisch and D.I. Kiener organized the Topical Session "Fundamentals of Fracture" at the DPG Spring Meeting 2023, Dresden (Germany), 26 - 31 Mar 2023

T. Hickel and S. Divinskyi organized the Topical Session "Defect Phases" at the DPG Spring Meeting 2023, Dresden (Germany), 26 - 31 Mar 2023

J. Neugebauer, T. Hickel and R. Drautz organized the Hands-on tutorial "Workflows in Materials Science Simulations" at the DPG Spring Meeting 2023, Dresden (Germany), 26 - 31 Mar 2023

J. Neugebauer, A. Perazzo, J. Schrier and P. Yang organized the "Workshop III: Complex Scientific Workflows at Extreme Computational Scales" at the IPAM Long Program "New Mathematics for the Exascale: Applications to Materials Science" at the University of California (USA), 1 - 5 May 2023

A. Saksena and B. Gault, organised the 9th NRW – Atom Probe Tomography user meeting at MPIE, Düsseldorf (Germany), 16 - 17 May 2023

M.J. Duarte, A. Lassnig and B.-S. Li organized the Symposium "Mechanical Properties and Adhesion" at the 49th International Conference on Metallurgical Coatings & Thin Films (ICMCTF 2024), San Diego, CA (USA), 21 - 26 May 2023

M. Rabe co-organized the "RESOLV 9th Summer School on Solvation Science" at ZEMOS, Bochum (Germany), 30 May - 02 Jun 2023

M. Rohwerder and M. Prabhakar organized the international meeting on Investigation and Modelling of Hydrogen Effusion in Electrochemically Plated Ultra-High-Strength-Steels used for Landing Gear Structures "H2Free" at the MPI-SusMat, Düsseldorf (Germany), 15 Jun 2023

T. Hickel, S. Menon and O. Waseda organized the Workshop: "Workflows for materials science simulations with pyiron" at the NFDI-MatWerk Conference, Hybrid Conference - Siegburg (Germany) & Online, 27 - 29 Jun 2023

M. Todorova, D. Jiang, G. Henkelmann and R. Hennig organized the "Computational Materials Chemistry Workshop", Telluride, Colorado (USA), 17 - 21 Jul 2023

M. Rohwerder organized the "Kick Off Coat4Hydrogen Meeting" at the MPI-SusMat, Düsseldorf (Germany), 14 Aug 2023

E. Bitzek, G. Dehm, C. Freysoldt, D. Raabe and M. Todorova organized the "New Horizons in Materials Design Workshop" at the MPI-SusMat, Düsseldorf (Germany), 17 - 18 Aug 2023

Y. Ma co-organized the Symposium "H10 - Fundamental Science of Sustainable Metallurgy" at EUROMAT 2023, Frankfurt am Main (Germany), 03 - 07 Sep 2023

E. Bitzek organized the SusMet Workshop "Research Data Management" at the MPI-SusMat, Düsseldorf (Germany), 22 Sep 2023

F. Stein co-organized the international conference "Intermetallics 2023" at the Educational Center Kloster Banz, Bad Staffelstein (Germany), 02 - 06 Oct 2023

M. Rohwerder organized the Symposium "C03 - Metallic, Organic, Inorganic, and Composite Coatings for Corrosion Protection" at the 244th ECS Meeting, Gothenburg (Sweden), 08 Oct 2023

M. Rohwerder organized the Symposium "C04 - Analytical Tools in Corrosion Research" at the 244th ECS Meeting, Gothenburg (Sweden), 08 Oct 2023

T. Hickel and J. Neugebauer organized "Ab initio Description of Iron and Steel (ADIS2023): Digitalization and Workflows" at the Ringberg Castle, Bavaria (Germany), 29 Oct - 03 Nov 2023

2024

M. Todorova and D. Holec organized the 4th German-Austrian Workshop "Computational Materials Science on Complex Energy Landscapes" in Kirchdorf (Austria), 15 - 19 Jan 2024

F. Stein and M. Palm co-organized the "8th MSIT Winter School on Materials Chemistry", at Ringberg Castle, Bavaria (Germany), 21 - 26 Jan 2024

G. Dehm, C. Scheu, B. Bellon, D. Sonawane and R. Sahu organized the Symposium "Mechanics Meets Energy 2024", Bad Neuenahr-Ahrweiler (Germany), 22 - 26 Jan 2024

P. Jovičević-Klug and C. Negi co-organized the event "Women in Science Week 2024" by M.S.C.A. Steminist in cooperation with young EFC, Alexander von Humboldt Foundation and Coatings Journal, held online, 05 - 09 Feb 2024

C. Liebscher co-organized the topical session "In situ and Multimodal Microscopy in Materials Physics" at the DPG Spring Meeting 2024, Berlin (Germany), 17 - 22 Mar 2024

T. Hickel, C. Pistidda and A. Punkdt organized the Topical Session "Hydrogen in Materials: from Storage to Embrittlement" at the 87th annual meeting of the German Physical Society (DPG Jahrestagung), Berlin (Germany), 17 - 22 Mar 2024

J. Neugebauer, T. Hickel and R. Drautz organized the Hands-on tutorial "Workflows in Materials Science" at the 87th annual meeting of the German Physical Society (DPG Jahrestagung), Berlin (Germany), 17 - 22 Mar 2024

J. Neugebauer and H. Springer organized the Topical Session "Sustainable Metallurgy" at the 87th annual meeting of the German Physical Society (DPG Jahrestagung), Berlin (Germany), 17 - 22 Mar 2024

A. Saksena, P. Bagot, X. Sauvage and B. Gault organised a Workshop Hydrogen Analysis by Atom Probe Tomography at MPI-SusMat (Germany), 16-18 April 2024

A. Saksena, T.M. Schwarz and B. Gault organised the 10th NRW – Atom Probe Tomography user meeting at MPI-SusMat, Düsseldorf (Germany), 19-21 May 2023

M.J. Duarte, A. Lassnig and B.-S. Li organized the Symposium "Mechanical Properties and Adhesion" at the 50th International Conference on Metallurgical Coatings & Thin Films (ICMCTF 2024), San Diego, CA (USA), 19 - 24 May 2024

M. Rabe and N. Samiseresht co-organized the "RESOLV Summer School on Solvation Science" at ZEMOS, Bochum (Germany), 21 - 24 May 2024

G. Dehm organized the Symposium "Metals and Alloys" at the European Microscopy Conference (EMC2024), Copenhagen (Denmark), 25 - 30 Aug 2024

T. Beck, G. Goldbeck and T. Hickel organized the Symposium "D03: Digital Materials: Experiments, simulation workflows, ontologies, and interoperability" at MSE2024, Darmstadt (Germany), 24 - 26 Sep 2024

C. Eberl, T. Hickel and M. Zimmermann organized the Symposium "D01: Navigating the Digital Revolution in Material Science and Engineering - General Symposium Topic D" at MSE2024, Darmstadt (Germany), 24 - 26 Sep 2024

Y. Ma co-organized the Symposium "I04 – Sustainable Synthesis and Processing of Metals" at MSE2024, Darmstadt (Germany), 24 - 26 Sep 2024

Institute colloquia and invited seminar talks

2022

Yuki Yamada, Osaka University, Osaka, Japan: Salt-concentrated liquid electrolytes: unique features and battery applications (05 Apr 2022)

Jennifer L.M. Rupp, Technical University of Munich & TUM International Energy, Munich, Germany: Design of Novel Hybrid and Solid State Battery Materials and Cell Prototypes (08 Apr 2022)

G. Jeffrey Snyder, Northwestern University in Evanston Illinois, USA: Engineering Grain Boundaries in Thermo-electric Materials (Apr 25 2022)

Chris Bumby, Victoria University of Wellington, Wellington, New Zealand: Hydrogen-DRI in New Zealand: Developing a process for the hydrogen reduction of titanomagnetite ironsand (27 Apr 2022)

Ran He, Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e. V. (IFW), Dresden, Germany: Half-Heusler thermoelectric materials: Towards the decoupling between electrons and phonons (28 Apr 2022)

Pingjun Ying, Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e. V. (IFW), Dresden, Germany: High performance Te-free thermoelectric materials and modules for Low-T applications (28 Apr 2022)

Christian Haug, Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany: Tribologically Induced Deformation Mechanisms and Friction as a Function of Crystal Orientation in Copper (27 Jun 2022)

Nicolas Combe, Centre national de la recherche scientifique (CNRS), Toulouse, France: Grain boundary-based plasticity: shear coupling migration and disconnections (12 Jul 2022)

Hongmin Zhu, Tohoku University and University of Science & Technology Beijing (USTB), Japan: Electrochemical approach for sustainable metallurgical process and recycling (12 Aug 2022)

Heung Nam Han, Seoul National University, Republic of Korea, Seoul, Republic of Korea: Mechanistic View on Electric Current Induced Kinetic Enhancement and its Various Examples in Materials (26 Sept 2022)

Bilge Yildiz, Massachusetts Institute of Technology (MIT), USA: Understanding and tuning the surface chemistry of perovskite oxides to activate oxygen exchange and water splitting reactions (4 Oct 2022)

Can Yildirim, European Synchrotron Radiation Facility ESRF, Grenoble, Auvergne-Rhône-Alpes, France: Dark Field X-ray Microscopy: A Synchrotron-based Rock'n Roll Imaging (07 Oct 2022)

Luciano Borasi, École polytechnique fédérale de Lausanne (EPFL) Lausanne, Switzerland: Bringing metal casting to microfabrication: process development and plastic deformation (28 Nov 2022)

Magdalena Ola Cichocka, Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e. V. (IFW), Dresden, Germany: Unraveling the structures of nanocrystalline materials by combining TEM and XRPD (16 Dec 2022)

Nicolas Perez Rodriguez, Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e. V. (IFW), Dresden, Germany: Transport and thermal measurements in the IMW-PPMS Lab (16 Dec 2022)

2023

Wangzhong Mu, Department of Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden: Sustainable metallurgy: current activities and potential collaborations (25 Jan 2023)

TERIGELE, Department of Metallurgy, Graduate School of Engineering, Tohoku University, Sendai, Japan: Synthesis of Ti-based fine powder using shuttle of disproportionation and proportionation reactions of titanium ions in molten salts (02 Mar 2023)

Teresa Perez-Prado, IMDEA Materials Institute, Madrid, Spain: Additive Manufacturing of Energy-Saving Materials (27 Mar 2023)

Srinivasan G. Srivilliputhur, University of North Texas, Denton, TX, USA: Bonding Environment in Alloys: implications for modeling diffusion, phase transformations, and mechanical properties (10 Apr 2023)

Isabella Gallino, Saarland University, Saarbrücken, Germany: Exploration of ultra-fast time scales in metallic glasses and crystals (10 May 2023)

Cinzia Peruzzi, Reishauer AG, Wallisellen, Switzerland: Combining polarized Raman spectroscopy and micro-pillar compression to study the anisotropic microscale compressive behavior of bone at high strain rates (17 May 2023)

Susan Sinnott, Penn State University, University Park, PA, USA: Materials chemistry with dynamic charge reactive potentials (01 Jun 2023)

Davide Vacirca, Université Sorbonne Paris Nord, France: Novel thin film high entropy alloys with tunable microstructure and enhanced mechanical properties (15 Jun 2023)

Gabrielle Tiphene, Ecole Centrale de Lyon, France: High-Temperature Scanning Indentation (HTSI): using in-situ Nanoindentation to quantify Recovery Kinetics (15 Jun 2023)

Piyush Jagtap, Indian Institute of Technology (IIT), Hyderabad, India: Real-time Wafer Curvature Stress Measurements to Understand Deposition and Post-Deposition Stresses in Thin Films (05 Jul 2023)

Bernd Gludovatz, University of New South Wales (UNSW), Sydney, Australia: Strength and Fracture Resistance in Multicomponent Alloys and Additive Manufactured Materials (10 Jul 2023)

Nagamani Jaya Balila, Indian Institute of Technology (IIT) Bombay, India: Micro-mechanisms of Deformation and Failure in Advanced High Strength Steels Unraveled through Full-Field Strain Mapping (12 Jul 2023)

Genna Monahan, University of Galway, Galway, Ireland: Uncovering the Mechanisms that Lead to Bone Fragility as the Disease Progresses in a Type-2 Zucker Diabetic Fatty (ZDF) Rat (31 Jul 2023)

Changlong Wang and Stuart Walsh, Monash University, Melbourne, Australia: Exploring Australia's Potential in the Emerging Hydrogen-Based Green Commodity Market (07 Aug 2023)

Sutatch Ratanaphan, King Mongkut's University of Technology, Thonburi, Thailand: There's plenty of Room at the (Grain) Boundary (31 Aug 2023)

Saya Ajito, Tohoku University, Sendai, Japan: Stability of electrochemical hydrogen charging into iron in an aqueous solution containing NH₄SCN (01 Sep 2023)

Ivan Cole, RMIT University, Melbourne, Australia: Effect of droplets on inhibitor performance for steel and galvanized steel (01 Sep 2023)

Hiroshi Kakinuma, Tohoku University, Sendai, Japan: Real-time hydrogen visualization system with high spatial and temporal resolutions: Imaging the preferential hydrogen permeation at grain boundaries of pure Ni (01 Sep 2023)

Luke Daly, Glasgow University, Glasgow, Scotland, UK: An atoms eye view of Solar System Evolution (15 Sep 2023)

Marc Geers, Eindhoven University of Technology, Eindhoven, Netherlands: High-resolution Micro-Plasticity in Advanced High-Strength Steels (06 Nov 2023)

Fan Zhang, U.S. Department of Commerce, National Institute of Standards and Technology (NIST), Gaithersburg, USA: Unraveling the Complexities of Advanced Manufacturing: Insights from Synchrotron X-rays (6 Nov 2023)

Michael J. Mills, Ohio State University, Columbus, USA: Local Phase Transformations: A New Creep Strengthening Mechanism in Ni-Base Superalloys (13 Nov 2023)

Vijayshankar Dandapani, Indian Institute of Technology Bombay, Bombay, India: Combined hydrogen potentiometry and electrochemical impedance spectroscopy approach for quantifying oxygen reduction reaction kinetics at buried organic coating/metal interfaces (14 Nov 2023)

Yuichi Ikuhara, University of Tokyo, Japan: Atomistic Dynamics of Deformation, Fracture and GB Migration in Oxides (12 Dec 2023)

2024

Berit Goodge, MPI for Chemical Physics of Solids, Dresden, Germany: Structure and Spectroscopy at the Atomic Scale: Advanced Electron Microscopy for improved Design of Functional Materials (11 Jan 2024)

Marc Willinger, Technical University of Munich (TUM), Garching, Germany: Observing while it happens: Operando Electron Microscopy in Catalysis Research (30 Jan 2024, Colloquium)

Women in Science Week, in collaboration with M.S.C.A. STEMinist, Coatings MDPI, youngEFC and Alexander von Humboldt Foundation (05 - 11 Feb 2024)

Markus Stricker, ICAMS, Ruhr-Universität Bochum (RUB), Bochum, Germany: Mesoscale Simulation of Grain Boundaries (15 Feb 2024)

Santhana Eswara, Luxembourg Institute of Science and Technology (LIST), Esch-sur-Alzette, Luxembourg: New in-situ and Operando Techniques for Correlative Microscopy and Chemical Imaging: Case Studies in Mapping Hydrogen and other low-Z Elements in Energy Materials (22 Feb 2024)

Sabina Markelj, Jožef Stefan Institute, Ljubljana, Slovenia: Deuterium Retention Studies in Displacement Damaged Tungsten in order to gain Understanding of the Phenomena involved to predict Fuel Retention in Future Devices (27 Feb 2024)

Michael Strebl, FAU Erlangen-Nürnberg, Erlangen, Germany: Respirometric Monitoring of Corrosion (28 Feb 2024)

Seung Min Jane Han, Korea Advanced Institute of Science and Technology (KAIST), Seoul, Republic of Korea and Technical University of Munich (TU), Munich Germany: Strengthening and Toughening Mechanisms in Metal-Graphene Nanolayered Composites (20 Mar 2024)

Silja-Katharina Rittinghaus, University of Wuppertal, Germany: Refractory Alloys and Composites - Pathways to Improved Performance (20 Mar 2024)

Gaurav Mohanty, Tampere University, Tampere, Finland: Constant Strain Rate Nanoindentation up to 10,000 s⁻¹ for Reliable Extraction of Mechanical Properties and Activation Parameters (25 Mar 2024)

Janez Zavašnik, Jozef Stefan Institute, Ljubljana, Slovenia: Sustainability and Raw Materials: Do we have them enough? (18 Apr 2024)

Ulla Weber, MPG: Gender Equality@Max Planck, in collaboration with PostdocNet Equality and Diversity WG (22 Apr 2024)

Astrid Pundt, Karlsruher Institut für Technologie (KIT), Karlsruhe, Germany: H in Thin Films: Size and Stress Effects on the System Thermodynamics and Kinetics (23 Apr 2024, Colloquium)



Cristina Vicente Manzano, Spanish National Research Council (CSIC), Madrid, Spain: Materials Grown by Electrochemical Techniques: The Route Towards Sustainable Materials for Energy (07 Jun 2024)

G. Jeffrey Snyder, Northwestern University, Evanston IL, USA: Defects and Grain Boundary Effects on Thermal and Electrical Transport (18 Jun 2024)

Yuan Yu, RWTH Aachen University, Aachen, Germany: Designing Thermoelectric Chalcogenides with Atom Probe Tomography (18 Jun 2024)

Christian Motz, Saarland University, Saarbruecken, Germany: Hydrogen Effects on the Deformation and Fracture of Alloys (18 Jun 2024, Colloquium)

Stefanus Harjo, J-PARC, Tokai, Japan: Microstructural characterization using pulsed neutron diffraction – stress, defects, texture, and phase transformations (19 Jun 2024)

Patricia Jovičević-Klug and Charu Negi, M.S.C.A. STEM-inist: STEM-inist Perspectives: Patricia and Charu with MSCA (10 Jul 2024)

Mark A. Buckingham, University of Manchester, Manchester, United Kingdom: Synthesis and Characterisation of High Entropy Metal Chalcogenides (11 Jul 2024)

Claudia Weidenthaler, Max-Planck-Institut für Kohlenforschung, Muelheim an der Ruhr, Germany: In situ Structure-Property Relationship Studies of Inorganic Catalysts for the Energy Transition (20 Aug 2024, Colloquium)

Richard Hennig, University of Florida, Gainesville, FL, USA: Accelerating the Discovery of Superconductors Through Deep Learning on Small Datasets (05 Sep 2024)

Cecile Deprez, DLR: Allyship: taking an active role against discriminations at work, in collaboration with Postdoc-Net Equality and Diversity WG (26 Sep 2024)

Alba Garzón Manjón, Institut Català de Nanociència i Nanotecnologia (ICN2), Barcelona, Spain: Real-Time Insights into Sustainable Materials: Correlative Electron Microscopy and Synchrotron Techniques (22 Oct 2024, Colloquium)

Lectures and teaching at universities

2021 (not included in Scientific Report 2019 - 2021)

Bitzek, E.; Ma, D.; Engel, M. Pre-course on Linux and Matlab (Block Lecture) (PrepLinux). FAU Erlangen-Nürnberg, WS 2021/2022

Bitzek, E.; Virtanen, S. Thermodynamics and Mechanics of Materials VL. FAU Erlangen-Nürnberg, WS 2021/2022

Bitzek, E. Seminar Thermodynamics and Mechanics of Materials. FAU Erlangen-Nürnberg, WS 2021/2022

Hickel, T. Introduction to Quantum Mechanics. Ruhr-Universität Bochum, WS 2021/2022

Neugebauer, J. Application and Implementation of Electronic Structure Methods. Ruhr-Universität Bochum, WS 2021/2022

Roters, F. Prozess- und Werkstoffsimulation. RWTH Aachen, WS 2021/2022

2022

Bitzek, E. Numerical Methods in Materials Science: Atomistic Simulations. FAU Erlangen-Nürnberg, SS 2022

Bitzek, E.; Zahn, D. Computational Nanoscience. FAU Erlangen-Nürnberg, SS 2022

Dehm, G.; Liebscher, C.; Zhang, S.; Scheu, C. Atomare Charakterisierung von Werkstoffen. Heinrich-Heine Universität Düsseldorf, WS 2022/2023

Dehm, G. Mechanische Eigenschaften in kleinen Dimensionen. Ruhr-Universität Bochum, SS 2022

Dehm, G. Transmissionselektronenmikroskopie für Fortgeschrittene. Ruhr-Universität Bochum, WS 2022/2023

Gault, B. Graduate course on Atom Probe Tomography, as part of the Centre for Doctoral Training on Materials Characterisation. Imperial College London, UK, SS 2022

Gault, B. 3rd year course on Engineering alloys (4h block lectures on advanced microscopy). Imperial College London, UK, SS 2022

Körmann, F. Introduction to Quantum Mechanics in Solid State Physics. Ruhr-Universität Bochum, WS 2022/2023

Liebscher, C. Transmissionselektronenmikroskopie für Fortgeschrittene (Übung). Ruhr-Universität Bochum, WS 2022/2023

Neugebauer, J. Application and Implementation of Electronic Structure Methods. Ruhr-Universität Bochum, WS 2022/2023

Raabe, D. Sustainable Materials Science and Green Metallurgy. RWTH Aachen, SS 2022

Rohwerder, M. Surface Science and Corrosion. Ruhr-Universität Bochum, WS 2022/2023

Roters, F. Prozess- und Werkstoffsimulation. RWTH Aachen, WS 2022/2023

Scheu, C. Moderne Material- und Werkstoffcharakterisierung: Vom Atom zum Bauteil. RWTH Aachen, SS 2022

Springer, H. Allgemeine Werkstofftechnik. RWTH Aachen, WS 2022/2023

Zaefferer, S.; Hickel, T.; Song, W. Microstructures, Microscopy and Modelling. RWTH Aachen, SS 2022

2023

Bitzek, E. Numerical Methods in Materials Science: Atomistic Simulations (Lecture and Computational Lab-Course). FAU Erlangen-Nürnberg, SS 2023

Dehm, G.; Liebscher, C.; Zhang, S.; Scheu, C. Atomare Charakterisierung von Werkstoffen. Heinrich-Heine Universität Düsseldorf, WS 2023/2024

Dehm, G. Mechanische Eigenschaften in kleinen Dimensionen. Ruhr-Universität Bochum, SS 2023

Dehm, G. Transmissionselektronenmikroskopie für Fortgeschrittene. Ruhr-Universität Bochum, WS 2023/2024

Gault, B. Graduate course on Atom Probe Tomography, as part of the Centre for Doctoral Training on Materials Characterisation. Imperial College London, UK, SS 2023

Gault, B. 3rd year course on Engineering alloys (6h block lectures on advanced microscopy Ti- and Ni-alloys). Imperial College London, UK, SS 2023

Hickel, T. Introduction to Quantum Mechanics for Solid State Physics. Ruhr-Universität Bochum, WS 2023/2024

Neugebauer, J. Application and Implementation of Electronic Structure Methods. Ruhr-Universität Bochum, WS 2023/2024

Raabe, D. Sustainable Materials Science and Green Metallurgy. RWTH Aachen, SS 2023

Rohwerder, M. Surface Science and Corrosion. Ruhr-Universität Bochum, WS 2023/2024

Roters, F. Prozess- und Werkstoffsimulation. RWTH Aachen, WS 2023/2024

Scheu, C. Electron Microscopy & Analytical Techniques. RWTH Aachen, WS 2023/2024

Scheu, C.; Zhang, S.; Materials Characterization. Ruhr-Universität Bochum & Universität Duisburg-Essen, WS 2023/2024

Scheu, C. Moderne Material- und Werkstoffcharakterisierung: Vom Atom zum Bauteil. RWTH Aachen, SS 2023

Springer, H. Allgemeine Werkstofftechnik. RWTH Aachen, WS 2023/2024

Springer, H. Metallurgie und Recycling Eisen und Stahl. RWTH Aachen, SS 2023

Springer, H. Process Metallurgy and Recycling Iron and Steel. RWTH Aachen, SS 2023

Springer, H. Sustainable Iron and Steelmaking. RWTH Aachen, WS 2023/2024

Springer, H. Vertiefung Metallurgie 1. RWTH Aachen, SS 2023

Springer, H. Vertiefung Metallurgie 2. RWTH Aachen, WS 2023/2024

Zaefferer, S.; Hickel, T.; Song, W. Microstructures, Microscopy and Modelling. RWTH Aachen, SS 2023

2024

Bitzek, E. Atomistic Modeling of Mechanical Behavior (Lecture and Computational Lab-Course). FAU Erlangen-Nürnberg, SS 2024

Dehm, G.; Liebscher, C.; Zhang, S.; Scheu, C. Atomare Charakterisierung von Werkstoffen. Heinrich-Heine Universität Düsseldorf, WS 2024/2025

Dehm, G. Mechanische Eigenschaften in kleinen Dimensionen. Ruhr-Universität Bochum, SS 2024

Dehm, G. Transmissionselektronenmikroskopie für Fortgeschrittene. Ruhr-Universität Bochum, WS 2024/2025

Gault, B. Graduate course on Atom Probe Tomography, as part of the Centre for Doctoral Training on Materials Characterisation. Imperial College London, UK, SS 2024

Neugebauer, J. Application and Implementation of Electronic Structure Methods. Ruhr-Universität Bochum, WS 2024/2025

Raabe, D. Sustainable Materials Science and Green Metallurgy. RWTH Aachen, SS 2024

Rohwerder, M. Die Zukunft sichern: Korrosionsforschung als ein wichtiger Faktor (Ringvorlesung). Ruhr-Universität Bochum, SS 2024

Roters, F. Prozess- und Werkstoffsimulation. RWTH Aachen, WS 2024/2025

Rohwerder, M. Surface Science and Corrosion. Ruhr-Universität Bochum, WS 2024/2025

Scheu, C. Moderne Material- und Werkstoffcharakterisierung: Vom Atom zum Bauteil. RWTH Aachen, SS 2024

Springer, H. Allgemeine Werkstofftechnik. RWTH Aachen, WS 2024/2025

Springer, H. Circular Metallurgy. RWTH Aachen, WS 2024/2025

Springer, H. Einführung Nachhaltige Werkstofftechnik. RWTH Aachen, WS 2024/2025

Springer, H. Metallurgie und Recycling Eisen und Stahl. RWTH Aachen, SS 2024

Springer, H. Process Metallurgy and Recycling Iron and Steel. RWTH Aachen, SS 2024

Springer, H. Sustainable Iron and Steelmaking. RWTH Aachen, WS 2024/2025

Springer, H. Vertiefung Metallurgie 1. RWTH Aachen, SS 2024

Springer, H. Vertiefung Metallurgie 2. RWTH Aachen, WS 2024/2025

Zaefferer, S.; Hickel, T.; Song, W. Microstructures, Microscopy and Modelling. RWTH Aachen, SS 2024

Invited talks at conferences and colloquia

2021 (not included in Scientific Report 2019 - 2021)

Bitzek, E.; Hickel, T.; Zimmermann, M.: *NFDI-MatWerk - an overview and discussion of the next steps* (Webinar MaterialsWeek2021. Online. 07 Sep. 2021)

Bitzek, E. *Mechanics at the Nanoscale: Comparison between Experiments and Simulations* (FAU NHR Atomistic Simulation Center (ASC) Inauguration Symposium 2021. Online. 26 Oct. 2021)

Bitzek, E.; Möller, J. J.; Baranova, P.; Lakshminpathy, T.; Eggle-Sievers, B.: *Atomistic Simulations of Crack-Microstructure Interactions in Metals* (1st (virtual) FRASCAL Symposium. Online. 26 Nov. 2021)

Brogna, A.; Best, J. P.; Djemia, P.; Faurie, D.; Dehm, G.; Ghidelli, M.: *Toward engineered thin film metallic glasses with large mechanical properties: effect of composition and nanostructure* (Seminar at Laboratoire des Sciences des Procédés et des Matériaux (LSPM), Paris Nord University. Paris, France. 17 Sep. 2021)

Garzón Manjón, A.: *Tailoring the structure and composition of complex solid solution nanoparticles for energy applications* (Seminar Series at Max Planck Institute for Solid State Research. Stuttgart, Germany. 04 Nov. 2021)

Liebscher, C.: *An atomic resolution view into the structural and chemical complexity of interfaces* (Modern electron microscopy and correlative techniques. Online. 06 Oct. 2021)

Stein, F.: *Diffusion Couples as a Tool for Materials Science* (Materials Science Special Seminar TU Freiberg. Virtual. 06 Dec. 2021)

Zhang, S.; Abdellaoui, L.; Bueno Villoro, R.; Scheu, C.; Luo, T.; Gault, B.; Raabe, D.: *Developing correlative and in situ microscopy to study structure-property relationships in thermoelectric materials* (Modern electron microscopy and correlative techniques. Online. 06 Oct. 2021)

2022

Aymerich Armengol, R.; Cignoni, P.; Ebbinghaus, P.; Rabe, M.; Tschulik, K.; Scheu, C.; Lim, J.: *Mechanism of coupled phase/morphology transformation of 2D manganese oxides through Fe galvanic exchange reaction* (Chemistry Department Seminar, Kangwon National University. Chuncheon, South Korea. 04 Aug. 2022)

Aymerich Armengol, R.; Cignoni, P.; Ebbinghaus, P.; Linnemann, J.; Rabe, M.; Tschulik, K.; Scheu, C.; Lim, J.: *Electron microscopy insights on the mechanism of morphology/phase transformations in manganese oxides* (Institut de Nanociència i Nanotecnologia (ICN2). Bellaterra, Spain. 16 Sep. 2022)

Best, J. P.: *Chemical segregation to grain boundaries: Probing the micromechanical response with site-specific in situ SEM measurements* (1st Materials Science Colloquium, 66. Metallkunde-Kolloquium of the Montanuniversität Leoben. Leoben am Arlberg, Austria. 19 Apr. 2022)

Best, J. P.; Tian, C.; Ma, Y.; Dehm, G.; Rasiński, M.: *Reduced toughness of recrystallised tungsten at grain boundaries evidenced through site-specific microcantilever fracture testing* (11th European Solid Mechanics Conference - ESMC 2022. Galway, Ireland. 04. Jul. 2022)

Best, J. P.: *The role of nanoscale structural ordering on the damage tolerance of laser-processed bulk metallic glasses* (Materials Science Engineering MSE 2022. Darmstadt, Germany. 27 Jul. 2022)

Best, J. P.: *Recent progress in micromechanical testing of grain boundaries* (Seminar at Laboratoire des Sciences des Procédés et des Matériaux (LSPM), Paris Nord University. Paris, France. 2022)

Bitzek, E.: *Elastic and Plastic Response of FCC-Metallic Nanostructures under complex Loads* (Gordon Research Conference Structural Nanomaterials. Les Diablerets, Switzerland. 08 May 2022)

Bitzek, E.: *The Origin of Deformation-Induced Topological Anisotropy in Silica Glass* (International Conference on the Strength of Materials ICSMA 19. Metz, France. 26 Jun. 2022)

Bitzek, E.: *Atomistic Simulations of Dislocation – Precipitate Interactions in Model Ni-based Superalloys* (EuroSuperalloys 2022 - 4th European Symposium on Superalloys and their Applications, Plenary. Bamberg, Germany. 18 Sep. 2022)

Bitzek, E.: *Atomistic Simulations, Mesoscale Modelling and Micromechanical Testing of Crack – Microstructure Interactions* (10th International Conference on Multiscale Materials Modeling MMM10. Baltimore, MD, USA. 02 Oct. 2022)

Brink, T.: *Thermodynamics of grain boundary phases in fcc metals: Using atomistic simulations to augment and extend experimental insights* (Materials Science Colloquium at the Technische Universität. Darmstadt, Germany. 08 Jun. 2022)

Brogna, A.; Best, J. P.; Djemia, P.; Faurie, D.; Dehm, G.; Ghidelli, M.: *Effect of composition and nanolayering on mechanical properties of Zr_{100-x}Cu_x thin film metallic glasses* (Talk at Université catholique de Louvain (UCL). Louvain-la-Neuve, Belgium. 02 Dec. 2022)

Bueno Villoro, R.: *Application of NbTiFeSb half Heusler thermoelectric materials* (Colloquium, Leibniz-Institut für Festkörper- und Werkstoffforschung. Dresden, Germany. 06 Oct. 2022)

Dehm, G.; Rao, J.; Duarte, M. J.: *Impact of Hydrogen on Dislocation Nucleation and Strength in bcc Fe–Cr alloys* (TMS 2022 Annual Meeting, Symposium “Mechanical Behavior at the Nanoscale VI.” Anaheim, CA, USA. 27 Feb. 2022)

Dehm, G.: *Grain Boundary Phases (Complexions) in Pure and Alloyed Cu: Insights from Advanced Electron Microscopy and Molecular Dynamics*. (Gordon Research Conference Structural Nanomaterials, Les Diablerets, Switzerland. 10 May 2022)

Dehm, G.: *Grain boundary phase transitions in pure and alloyed Cu* (Possibilities and Limitations of Quantitative Materials Modeling and Characterization 2022. Bernd-kastel-Kues, Germany. 22 May 2022)

Dehm, G.: *Structure and properties of tilt grain boundaries in Cu thin films* (Graduiertenkollegs GRK1896 „In situ microscopy with electrons, X-rays and scanning probes: Abschluss-symposium. Erlangen, Germany. 23 Jun. 2022)

Dehm, G.; Ahmadian, A.; Schreiber, D.; Zhou, X.; Gault, B.; Liebscher, C.; Romaner, L.: *Multi-Element Segregation at Bcc Iron Grain Boundaries and Their Impact on Mechanical Properties* (ELMINA2022. Belgrade, Serbia. 22 Aug. 2022)

Dehm, G.: *New insights on the atomic grain boundary structure in pure and alloyed Cu and Fe* (10th International Workshop on Interfaces. Santiago de Compostela, Spain. 04 Sep. 2022)

Dehm, G.; Langenohl, L.; Bishara, H.; Brink, T.; Liebscher, C.: *Atomic structure and phase stability of Cu tilt grain boundaries resolved by scanning transmission electron microscopy* (Materials Science and Engineering MSE Congress. Darmstadt, Germany. 27 Sep. 2022)

Dehm, G.; Jentner, R.; Best, J.; Kirchlechner, C.: *Challenges in The Phase Identification of Steels Using Unsupervised Clustering of Nanoindentation Data* (Nanomechanical Testing in Materials Research and Development VIII. Split, Croatia. 05. Oct. 2022)

Duarte, M.J.; Rao, J.; Dehm, G.: *Hydrogen and Micro-mechanics: case study of bcc Fe-Cr alloys during in situ hydrogen charging* (11th European Solid Mechanics Conference - ESMC 2022. Galway, Ireland. 07. Jul. 2022)

Duarte, M.J.; Rao, J.; Lee, S.; Gopalan, H.; Scheu, C.; Dehm, G.: *In situ micromechanics during hydrogen charging: Effect of diffusible hydrogen on bcc Fe-based alloys and hydrogen protection through barrier coatings* (Nanomechanical Testing in Materials Research and Development VIII. Split, Croatia. 02 Oct. 2022).

Fischer, A.: *Wear Scars do not represent Wear Loss – A Fretting Corrosion Example* (7th World Tribology Congress WTC 2022. Lyon, France. 14 Jul. 2022)

Freysoldt, C.; Gake, T.; Kumagai, Y.; Oba, F.; Dou, B.; Falletta, S.: *Charge corrections for electronic transitions at defects with ionic and electronic screening* (Workshop “First-principles modeling of defects in solids: Charges meet lattices.” Zürich, Switzerland. 13 Jun. 2022)

Garzón Manjón, A.: *Tailoring the structure and composition of complex solid solution nanoparticles for energy applications* (5th International Caparica Symposium on Nanoparticles/Nanomaterials and Applications 2022. Caparica, Portugal. 24 Jan. 2022)

Garzón Manjón, A.: *Highly active complex solid solution electrocatalysts for oxygen reduction reaction: characterization of the structure-activity correlations by (scanning) transmission electron microscopy* (Department of Materials & Earth Sciences, Technical University Darmstadt. Darmstadt, Germany. 02 May 2022)

Garzón Manjón, A.: *Highly active complex solid solution electrocatalysts for oxygen reduction reaction: characterization of the structure-activity correlations by (scanning) transmission electron microscopy* (Catalan Institute of Nanoscience and Nanotechnology (ICN2). Bellaterra, Barcelona, Spain. 04 Jul. 2022)

Gault, B.: *Facilitating routine nanoscale analysis of battery anode and cathode materials by using (cryo-) atom probe tomography* (2nd Energy Landscapes and Structure in Ion Conducting Solids (ELSICS) Workshop and International Bunsen-Discussion-Meeting. Göttingen, Germany. 26 Sep. 2022)

Gault, B.: *Cryo-atom probe tomography analysis of batteries* (Atom Probe Tomography & Microscopy 2022. Online. 11 Oct. 2022)

Gault, B.: *Forays into cryo-atom probe tomography of battery materials* (14th International Symposium on Atomic Level Characterizations for New Materials and Devices. Online. 16 Oct. 2022)

Hickel, T.; Grabowski, B.; Körmann, F.; Glensk, A.: *Application of Density Functional Theory in the Context of Phase Diagram Modelling* (6th MSIT Winter School, online. 05 Apr. 2022)

Hickel, T.; Janssen, J.; Sözen, H.; Sreekala, L.; Körmann, F.; Surendralal, S.; Todorova, M.; Neugebauer, J.: *High-throughput optimization of finite temperate Phase stabilities: Concepts and application* (PTM 2022, virtual conference. 30 Jun. 2022)

Hickel, T.; Sözen, H.; Hegde, O.; Waseda, O.; Körmann, F.; Janßen, J.; Neugebauer, J.: *Design of finite temperature materials properties enabled by innovative digital concepts* (Allgemeines Physikalisches Kolloquium, Physik-Institute of Münster University, Germany. 28 Apr. 2022.)

Hickel, T.; Sözen, H.; Hegde, O.; Waseda, O.; Körmann, F.; Janßen, J.; Neugebauer, J.: *pyron - an integrated development Environment for Workflows in materials science* (FONDA data science workshop, Humboldt-Universität zu Berlin, Germany. 12 May 2022)

Hickel, T.; Sözen, H.; Hegde, O.; Waseda, O.; Körmann, F.; Janßen, J.; Neugebauer, J.: *Workflow Management in advanced materials science* (Bielefelder Tag der Materialforschung, Hochschule Bielefeld (HSBI), Germany. 27 Sep. 2022)

Hickel, T.; Sözen, H.; Sreekala, L.; Hegde, O.; Janßen, J.; Neugebauer, J.: *Ab initio thermodynamics of magnetic materials* (HetSys PX918 Seminar, Warwick University, UK. 07 Nov. 2022)

Jentner, R.; Best, J. P.; Kirchlechner, C.; Dehm, G.: *Challenges in the phase identification of steels using unsupervised clustering of nanoindentation data* (Nanomechanical Testing in Materials Research and Development VIII. Split, Croatia. 02 Oct. 2022)

Jung, C.: *Nanostructuring of NbCoSn-based half-Heusler thermoelectric materials through the crystallization of an amorphous precursor* (Colloquium, Leibniz-Institut für Festkörper- und Werkstofforschung. Dresden, Germany. 06 Oct. 2022)

Kasdorf Giesbrecht, C.; Rohwerder, M.: *Gold Electrodes Emerged from Aqueous Electrolytes: A Kelvin Probe and Infrared Spectroscopy Approach* (241st ECS Meeting. Vancouver, Canada. 29 May 2022)

Kusampudi, N.; Diehl, M.: *Inverse design of dual-phase steel microstructures using generative machine learning model and Bayesian optimization* (Working Group Microstructural Mechanics, Deutsche Gesellschaft für Materialkunde e.V., Applications of Machine Learning for Mechanical Behavior of Materials. Online. 16 Nov. 2022)

Liebscher, C.: *High Entropy Materials* (Themenfeldtag Material BAM. Berlin, Germany. 27 Apr. 2022)

Liebscher, C.: *Grain Boundary Phase Transformations and Segregation Transitions in Metallic Alloys* (Grain Boundaries: Challenges and Opportunities, Workshop BAM. Berlin, Germany. 21 Oct. 2022)

Liebscher, C.: *Interface Phases in Metallic Alloys* (Werkstoffkunde Kolloquium KIT. Karlsruhe, Germany. 25 Oct. 2022)

Lymerakis, L.: *Ab-initio based investigations III-Nitride surfaces: Implications of growth conditions on alloy compositional limits* (The 3rd International Workshop on Materials Science and Advanced Electronics Created by Singularity/The 2nd International Symposium on Wide Gap Semiconductor Growth, Process and Device Simulation, Nagoya Congress Center (Japan) + Online. Hybrid event format. 11 Jan. 2022)

Ma, Y.; Wang, Y.-F.; Bugelnig, K.; Tsai, S.-P.; Villanova, J.; Zaefferer, S.; Requena, G.; Raabe, D.: *Microstructure and porosity evolution during hydrogen-based direct reduction of iron ore* (DGM X-ray tomography working group meeting. Online. 05 May 2022)

Ma, Y.: *Microstructure evolution during hydrogen-based direct reduction of iron oxides* (International Workshop on Sustainable Metallurgy of Green Steel (Green-Steel2022). Online. 12 Sep. 2022)

Ma, Y.; Wang, Y.-F.; Bugelnig, K.; Villanova, J.; Requena, G.; Raabe, D.: *Green steel: porosity evolution during hydrogen-based direct reduction of hematite probed by in-situ synchrotron X-ray nano-tomography* (MSE 2022. Darmstadt, Germany. 27 Sep. 2022)

Neugebauer, J.; Zendegani, A.; Hickel, T.: *Construction and Application of Defect Phase Diagrams* (TMS Annual Meeting and Exhibition. Anaheim, CA, USA. 27 Feb. 2022)

Neugebauer, J.; Hickel, T.; Körmann, F.; Todorova, M.: *Materials design and discovery in high-dimensional chemical and structural configuration spaces* (Psi-k 2020 Conference. Lausanne, Switzerland. 22 Aug. 2022)

Neugebauer, J.; Hickel, T.; Körmann, F.; Todorova, M.: *Materials design and discovery in high-dimensional chemical and structural configuration spaces* (International Conference on Materials Science, Engineering & Technology (Keynote talk). Singapore, Singapore. 07 Sep. 2022)

Neugebauer, J.; Huber, L.; Holec, D.; Gehring, D.; Hickel, T.: *Defect Phase Diagrams: Concepts, Computational Approaches and Materials Design Strategies* (MMM10 Conference. Baltimore, MD, USA. 07 Sep. 2022)

Neugebauer, J.; Surendralal, S.; Deibenbeck, F.; Wippermann, S. M.; Todorova, M.: *Surface adsorption under UHV conditions and in an electrochemical environment: An ab initio based comparison* (73rd Annual Meeting of the International Society of Electrochemistry. Virtual. 12 Sep. 2022)

Raabe, D.; Souza Filho, I. R.: *Green Steel Research at the Max Planck Institute* (Webinar Green Steel, Arcelor Mittal Brazil. Online. 15 Feb. 2022)

Raabe, D.: *Mechanisms behind hydrogen-based green steel making* (PICO 2022 Conference. Vaalsbroek, The Netherlands. 10 May 2022)

Raabe, D.: *Sustainable Metals for a Circular Economy* (The Morris E. Fine Lecture at Northwestern University. Evanston, IL, USA. Virtual. 31 May 2022)

Ramachandramoorthy, R.: *Pushing the boundaries of microfabrication and micromechanics* (Indian Institute of Metals lecture, Indian Institute of Technology Madras. Chennai, India. 20 Apr. 2022)

Ramachandramoorthy, R.: *Micro and Nanomechanics at high strain rates* (Platinum Jubilee Lecture - Indian Institute of Science. Bengaluru, India. 28 Apr. 2022)

Ramachandramoorthy, R.: *Fabrication and dynamic testing of full-metal microarchitectures* (European Solid Mechanics Conference. Galway, Ireland. 05 Jul. 2022)

Ramachandramoorthy, R.: *Electrodeposition meets small-scale mechanics: Fabrication and destruction* (Max-Planck Chemistry, Physics and Technology Section Symposium. Berlin, Germany. 20 Oct. 2022)

Rao, Z.; Tung, P.-Y.; Xie, R.; Zhang, H.; Wei, Y.; Li, Z.; Gutfleisch, O.; Bauer, S.; Raabe, D.: *Machine learning-enabled fast high-entropy alloy discovery - a case study on novel Invar alloys* (DGM workshop: Functional High Entropy Alloys / Hochentropiefunktionswerkstoffe. Bochum, Germany. 29 Mar. 2022)

Rohwerder, M.: *Measuring Hydrogen Permeation and Effusion by Kelvin Probe-Based Techniques: New Insights into Limitations and Possibilities* (Gordon Research Conference 2022 on Aqueous Corrosion (Keynote Lecture). New London, NH, USA. 10 Jul. 2022)

Rohwerder, M.: *Kelvin probe based methods for measuring effusion and diffusion of hydrogen from and through materials at high resolution and sensitivity* (13th International Symposium on Electrochemical Methods in Corrosion Research (EMCR). St Pierre d'Oléron, France. 25 Sep. 2022)

Scheu, C.: *Interfaces in functional materials: what can we learn from combining APT and TEM* (PICS 2022. Marseilles, France. 02 Jun. 2022)

Scheu, C.: *Tracing impurities and structural defects in energy materials using advanced scanning transmission electron microscopy and atom probe tomography* (Retreat Lotsch Group, Germany, Schloss Fürstenried, Germany. 13 Jun. 2022)

Scheu, C.: *Insight in the structure and stability of (photo) catalysts* (Graduiertenkollegs GRK1896 „In situ microscopy with electrons, X-rays and scanning probes: Abschluss-symposium. Erlangen, Germany. 23 Jun. 2022)

Scheu, C.; Abdellaoui, L.; Bueno Villoro, R.; Cojocaru-Mirédin, O.; Gault, B.; Luo, T.; Jung, C.; Yu, Y.; Zaefferer, S.; Zhang, S.: *A scale bridging approach for analysis of extended defects in thermoelectric materials: From electron channeling contrast imaging, scanning transmission electron microscopy to atom probe tomography* (ELMI-NA2022. Belgrade, Serbia. 22 Aug. 2022)

Scheu, C.: *Unravelling secrets of interfaces in renewable energy application* (10th International Workshop on Interfaces. Santiago de Compostela, Spain. 04 Sep. 2022)

Todorova, M.; Surendralal, S.; Wippermann, S. M.; Deißenbeck, F.; Neugebauer, J.: *Insights into processes at electrified solid/liquid interfaces from ab initio molecular dynamics simulations* (CMWS Water in Energy Research and Technology workshop, DESY, Hamburg, Germany. Online. 02 Mar. 2022)

Todorova, M.; Surendralal, S.; Yoo, S.-H.; Wippermann, S. M.; Deißenbeck, F.; Neugebauer, J.: *Ab initio insights into processes at solid/liquid interfaces* (Workshop on the "Fundamentals of the electrochemistry of the metal/electrolyte interface." London, UK. 06 Jul. 2022)

Todorova, M.; Surendralal, S.; Deißenbeck, F.; Wippermann, S. M.; Neugebauer, J.: *The role of water at electrified solid/liquid under potential control* (Psi-k 2020 Conference. Lausanne, Switzerland. 22 Aug. 2022)

Todorova, M.; Surendralal, S.; Deißenbeck, F.; Wippermann, S. M.; Neugebauer, J.: *The role of water at electrified solid/liquid Interfaces under potential control* (Materials Science, Engineering & Technology International Conference. Singapore, Singapore. 07 Sep. 2022)

Todorova, M.; Surendralal, S.; Wang, Z.; Deißenbeck, F.; Wippermann, S. M.; Neugebauer, J.: *Insights into Electrified Solid/Liquid Interfaces from Ab initio and Atomistic Molecular Dynamics Simulations* (73th Annual Meeting of the International Society of Electrochemistry (Keynote talk). Online. 12 Sep. 2022)

Vega Paredes, M.; Arenas Esteban, D.; Garzón Manjón, A.; Scheu, C.: *How can electron tomography be used for studying the catalyst degradation of fuel cells* (Advanced Electron Nanoscopy Group – Institut Catala de Nanociencia I Nanotecnologia. Bellaterra, Spain. 22 Nov 2022)

Zhang, S.; Mingers, A. M.; Kim, S.-H.; Kasian, O.; Cherevko, S.; Gault, B.; Scheu, C.: *Operando study on the activation and corrosion of (photo)electrocatalysts* (Colloquium, Ludwig-Maximilians-Universität. München, Germany. 14 Jun. 2022)

Zhang, S.; Kim, S.-H.; Mingers, A. M.; Gault, B.; Scheu, C.: *Operando study on the activation and corrosion of (photo)electrocatalysts* (Colloquium, Walter Schottky Institut. München, Germany. 15 Jun. 2022)

Zhang, S.; Abdellaoui, L.; Bueno Villoro, R.; Jung, C.; Matlat, D. A.; Scheu, C.: *In situ microstructural observation of PbTe thermoelectrics by TEM* (Colloquium, Leibniz-Institut für Festkörper- und Werkstoffforschung. Dresden, Germany. 06 Oct. 2022)

2023

Aymerich Armengol, R.: *Stability of 2D oxide and chalcogenide nanomaterials under synthesis and application conditions* (MRSEC Seminar Series, Northwestern University. Evanston, IL, USA. 14 Mar. 2023)

Aymerich Armengol, R.: *Understanding the stability of nanomaterials through electron microscopy techniques* (Physics Department, Technical University of Denmark. Kongens Lyngby, Denmark. 24 May 2023)

Aymerich Armengol, R.: *Determination of the structural and electrochemical stability of nanocatalysts for electrolyzer applications* (Chemistry Department, Kangwon National University. Chuncheon-si, South Korea. 08 Sep. 2023)

Aymerich Armengol, R.: *Techniques for the assessment of the stability of (sea) water splitting nanocatalysts* (Korean Institute for Energy Research. Jeju, South Korea. 18 Sep. 2023)

Best, J. P.: *Exploring the links between local chemistry and nano-/microscale deformation using in situ testing* (ScopeM Seminar, ETH. Zürich, Switzerland. 16 Jul. 2023)

Bhatt, S.; Katnagallu, S.; Freysoldt, C.; Neugebauer, J.: *DFT study on field ion microscopy contrast* (Invited Seminar, Rouen University, Rouen, France. 6 Feb. 2023)

Bitzek, E.: *Challenges to (Multiscale) Modelling of Fracture in Metals and Alloys* (2nd FRASCAL Symposium. Erlangen, Germany. 15 Mar. 2023)

Bitzek, E.: *Elastic and Plastic Response of FCC-Metallic Nanostructures under complex Loads* (MecaNano General Meeting. Madrid, Spain. 22 Apr. 2023)

Bitzek, E.: *Dislocation-mediated Plasticity with a focus on size effects* (MecaNano Summer School on Experimental Nano- and Micromechanics. Rome, Italy. 24 Jul. 2023)

Bitzek, E.: *Atomistic Simulations, Mesoscale Modelling and Micromechanical Testing of Crack – Microstructure Interactions* (XVII International Conference on Computational Plasticity, Fundamentals and Applications (COMPLAS 2023). Barcelona, Spain. 05 Sep. 2023)

Bitzek, E.: *Towards High-Throughput Atomistic Microstructure – Mechanics Simulations* (Ab initio Description of Iron and Steel (ADIS2023): Digitalization and Workflows. Schloss Ringberg, Tegernsee, Germany. 29 Oct. 2023)

Brink, T.: *Atomistic simulations of grain boundary phases: From thermodynamics to mechanics* (Seminar Materials Science and Technology at the RUB. Bochum, Germany. 02 Feb. 2023)

Brink, T.; Pemma, S.; Langenohl, L.; Ahmad, S.; Liebscher, C.; Dehm, G.: *Complexions in fcc metals: Insights from atomistic simulations* (2nd Materials Science Colloquium. Lech am Arlberg, Austria. 17 Apr. 2023)

Brink, T.; Langenohl, L.; Ahmad, S.; Liebscher, C.; Dehm, G.: *Atomistic Modeling of the Thermodynamics of Grain Boundaries in fcc Metals* (19th International Conference on Diffusion in Solids and Liquids. Crete, Greece. 26 Jun. 2023)

Bueno Villoro, R.: *Effect of grain boundary phases on the properties of half Heusler thermoelectrics* (Northwestern University. Evanston, IL, USA. 13 Mar. 2023)

Bueno Villoro, R.: *Electron microscopy investigations to understand the transport properties of energy materials* (Physics Department, Technical University of Denmark. Kongens Lyngby, Denmark. 24 May 2023)

Cheng, N.: *In situ transmission electron microscopy study of functional nanomaterials* (Catalan Institute of Nanoscience and Nanotechnology. Barcelona, Spain. 14 Jul. 2023)

Dehm, G.: *Grain Boundaries: An "old" Defect Gaining New Momentum in Materials Science* (Seminarvortrag an der EPFL Lausanne. Online. 27 Mar. 2023)

Dehm, G.: *Can we prevent Zn induced liquid metal embrittlement in steel by grain boundary segregation?* (PICS 2023. Marseilles, France. 02 May 2023)

Dehm, G.: *On the interplay between grain boundary complexions and chemical composition for fcc metals* (Possibilities and Limitations of Quantitative Materials Modeling and Characterization 2023. Bernkastel-Kues, Germany. 14 May 2023)

Dehm, G.: *Probing defect - defect interactions in metals and (complex) alloys by in-situ nanomechanics* (Nano-Brücken 2023: Nanomechanical Testing Conference. Saarbrücken, Germany. 23 May 2023)

Dehm, G.: *Grain boundary phases in metallic materials: Structure, stability and properties* (MiFuN III - Microstructural Functionality at the Nanoscale. Venice, Italy. 08 Jun. 2023)

Dehm, G.; Langenohl, L.; Ahmad, S.; Ahmadian, A.; Frolov, T.; Duarte, M. J.; Richter, G.; Zhou, X.; Gault, B.; Bishara, H.; Brink, T.; Liebscher, C.: *Resolving grain boundary complexions in Copper by STEM and analyzing their impact on properties* (Workshop Advanced Electron Microscopy in Materials Research. La Clusaz, France. 15 Jul. 2023)

Dehm, G.; Liebscher, C.: *In situ TEM study of deformation and phase transformation mechanisms in chemically complex alloys* (Symposium In-situ & Environmental Microscopy, 20th International Microscopy Congress. Busan, Korea. 13 Sep. 2023)

Dehm, G.: *Resolving the interplay of structure and energy landscapes of tilt grain boundaries in metals* (3rd ELSICS Conference and Bunsen-Colloquium "Energy Landscapes and Structure in Ion Conducting Solids (EL-SICS)." Ulm, Germany. 04 Oct. 2023)

Dehm, G.; Scheu, C.; Gopalan, H.; Hieke, S. W.; Duarte, M. J.: *Stability of Amorphous Al₂O₃ Hydrogen Barrier Coatings during Application* (The International Symposium on Advanced Coatings for Energy – ISC4E 2023. Ben Guerir, Morocco. 27 Nov. 2023)

Duarte, M.J.; Rao, J.; Lee, S.; Gopalan, H.; Scheu, C.; Dehm, G.: *Micromechanics during hydrogen charging: Instrumentation development and diffusive hydrogen* (KLA Nanoindentation User Meeting, Europe. Technical University Darmstadt. Darmstadt, Germany. 8 Mar. 2023).

Freysoldt, C.; Hennig, R. G.; Neugebauer, J.: *Ab initio calculations of charged defects at surfaces* (APS March Meeting 2023. Las Vegas, NV, USA. 05 Mar. 2023)

Freysoldt, C.: *Exploring data-rich materials analytics with machine learning: how and why* (Physikalisches Kolloquium, Philipps-Universität. Marburg, Germany. 03 May 2023)

Freysoldt, C.; Wang, N.; Sreekala, L.; Bukka, S. R.; Goyal, P. K.; Liebscher, C.; Saxena, A.; Gault, B.: *Pattern discovery and quantification in experimental data from scanning transmission electron tomography (STEM) and atom probe tomography (APT)* (Big Max Summer School. Cap Roig, Spain. 25 May 2023)

Freysoldt, C.; Saxena, A.; Wang, N.; Sreekala, L.: *Perspectives for machine learning applied to data-rich experiments on complex materials* (Materials Chain International Conference. Bochum, Germany. 31 Aug. 2023)

Freysoldt, C.; Katnagallu, S.; Bhatt, S.; Saxena, A.; Ashton, M. W.: *Pushing the limits of APT and FIM by pushing theoretical approaches* (APT & M 2023. Leuven, Belgium. 17 Sep. 2023)

Gong, Y.: *Synergy between Experimentation and Modeling for Life-time Prediction and Design against Corrosion* (Gordon Research Conference in High Temperature Corrosion: Degradation Mechanisms, Life Prediction and Improved Materials for Application in Extreme Environments. New London, NH, USA. 16 Jul. 2023)



Hickel, T.; Sözen, H. I.; Hegde, O.; Neugebauer, J.: *Design of finite temperature materials properties enabled by digital concepts* (HetSys Seminar Warwick University. Warwick, UK. 01 Jan. 2023)

Hickel, T.; Grabowski, B.; Körmann, F.; Menon, S.: *Application of density functional theory in the context of phase diagram modelling* (7th MSIT Winter School. Schloß Ringberg, Tegernsee, Germany. 13 Mar. 2023)

Hickel, T.; Zendegani, A.; Tehranchi, A.; Hegde, O.; Mathews, P.; Neugebauer, J.: *Constructing defect phase diagrams from ab initio calculations* (Fritz-Haber-Institut Seminar. Berlin, Germany. 23 Mar. 2023)

Hickel, T.; Schaarschmidt, J.; Straumal, A.: *The Platform MaterialDigital (PMD) and the goal of a Materials Data Space* (4th EMMC International Workshop 2023. 26 Apr. 2023)

Hickel, T.; Tehranchi, A.; Mathews, P.; Zendegani, A.; Zhang, S.; Scheu, C.; Neugebauer, J.: *Constructing defect phase diagrams from ab initio calculations* (6th MoD-PMI 2023 Workshop. Aachen, Germany. 29 Mai 2023)

Hickel, T.; Tehranchi, A.; Mathews, P.; Zendegani, A.; Zhang, S.; Scheu, C.; Neugebauer, J.: *Ab initio Thermodynamics of defect phases in metals* (19th Int. Conference on Diffusion in Liquids and Solids. Heraklion, Greece. 27 Jun. 2023)

Hickel, T.; Tehranchi, A.; Mathews, P.; Zendegani, A.; Zhang, S.; Scheu, C.; Neugebauer, J.: *Constructing defect phase diagrams from ab initio calculations* (Birmingham University, Seminar in physical chemistry. Birmingham, UK. 21 Jul. 2023)

Hickel, T.: *Research data infrastructures as enablers for materials design* (MCIC 2023 - 5th Materials Chain International Conference. Bochum, Germany. 31 Aug. 2023)

Hickel, T.; Sözen, H. I.; Hegde, O.; Janssen, J.; Neugebauer, J.: *Design of finite temperature materials properties enabled by digital concepts* (FEMS Euromat Conference 2023. Frankfurt a. Main, Germany. 03 Sep. 2023)

Hickel, T.; Waseda, O.; Huber, L.; Menon, S.; Janssen, J.; Drautz, R.; Neugebauer, J.: *Integration of multi-scale workflows into the pyiron IDE* (FEMS Euromat Conference 2023. Frankfurt a. Main, Germany. 03 Sep. 2023)

Hickel, T.; Tehranchi, A.; Chakraborty, P.; Lopez Freixes, M.; Zhao, H.; Gault, B.; Neugebauer, J.: *Defect-hydrogen interaction in Al alloys: Challenges and benefits revealed by ab initio calculations* (International hydrogen conference 2023. Park City, UT, USA. 18 Sep. 2023)

Hickel, T.; Tehranchi, A.: *Hydrogen enhances cross-slip of dislocations in the vicinity of grain boundaries* (International hydrogen conference. Park City, UT, USA. 19 Sep. 2023)

Hickel, T.: *Research data infrastructures as enablers for materials design* (MLEdays TUHH 2023. Hamburg, Germany. 25 Sep. 2023)

Janssen, J.; Neugebauer, J.: *Rapid prototyping and up-scaling atomistic workflows with pyiron* (Workshop "Ab initio Description of Iron and Steel (ADIS): Digitalization and Workflows". Schloß Ringberg, Tegernsee, Germany. 30 Oct. 2023)

Jung, C.: *Atom probe tomography for nanoscale characterization of functional materials* (Global Photovoltaic Conference 2023, Session: CiS. II-VI & Chalcogenide compound-based cells and materials, Satellite-CiS-2. Gwangju, Republic of Korea. 08 Sep. 2023)

Jung, C.: *Understanding of functional materials through atom probe analysis* (The 20th International Microscopy Congress, Workshop session for cryo atom probe tomography. Busan, Republic of Korea. 10 Sep. 2023)

Jung, C.: *Advanced characterization for functional materials* (Korea Institute of Materials Science. Changwon, South Korea. 11 Sep. 2023)

Jung, C.: *NbCoSn half-Heusler compounds through crystallization of amorphous precursors* (Korea Institute of Ceramic Engineering and Technology. Jinju, South Korea. 14 Sep. 2023)

Jung, C.: *Sample preparation of nanomaterials for atom probe analysis* (NRF-DFG meeting "Electrodes for direct sea-water splitting and microstructure based stability analyses", Korean Institute for Energy Research. Jeju, South Korea. 18 Sep. 2023)

Jung, C.: *Advanced characterization for functional nanomaterials* (Korea University. Seoul, South Korea. 22 Sep. 2023)

Jung, C.: *Sample preparation of nanomaterials for atom probe tomography* (Hanbat National University. Daejeon, South Korea. 25 Sep. 2023)

Jung, C.: *Atom probe tomography for nanostructured functional materials* (Korea Institute of Energy Research. Daejeon, South Korea. 26 Sep. 2023)

Jung, C.: *NbCoSn based half-Heusler compounds through crystallization of amorphous precursors* (Kyungpook National University. Daegu, South Korea. 16 Nov. 2023)

Jung, C.: *Investigation of interface between CIGS and buffer layer using atom probe tomography* (Korea Institute of Energy Research. Daejeon, South Korea. 29 Nov. 2023)

Jung, C.: *Understanding of the property-structure relationship for thermoelectric materials through advanced characterization* (Korea Electrotechnology Research Institute. Changwon, South Korea. 30 Nov. 2023)

Kruzic, J. J.; Li, B.; Gludovatz, B.; Nomoto, K.; Ringer, S. P.; Gammer, C.; Hohenwarter, A.; Eckert, J.; Best, J. P.: *Relating nanoscale structure and properties to macro-scale fracture toughness for bulk metallic glasses* (15th International Conference on Fracture. Atlanta, GA, USA. 11 Jun. 2023)

Liebscher, C.; Lu, W.; Langenohl, L.; Dehm, G.; Raabe, D.; Li, Z.: *Dynamic Observations of Complex Alloys and Interfaces by in situ S/TEM* (Microscopy Conference 2023. Darmstadt, Germany. 27 Feb. 2023)

Liebscher, C.: *Direct Observations of Grain Boundary Phase Transformations in Metallic Alloys* (DPG Spring Meeting 2023. Dresden, Germany. 29 Mar. 2023)

Liebscher, C.: *Grain Boundary Phase Transformations and Segregation Transitions in Metallic Alloys* (19th International Conference on Diffusion in Solids and Liquids. Crete, Greece. 26 Jun. 2023)

Liebscher, C.; Ahmadian, A.; Scheiber, D.; Zhou, X.; Darvishi, R.; Romaner, K. L.; Dehm, G.: *On the Role of Interstitial Solutes on Grain Boundary Segregation and Embrittlement in Ferritic Iron* (Thermec 2023 - International Conference on Processing & Manufacturing of advanced Materials. Vienna, Austria. 06 Jul. 2023)

Ma, Y.; Wang, Y.-F.; Bugelnig, K.; Villanova, J.; Requena, G.; Raabe, D.: *Porosity evolution during sustainable iron-making with hydrogen probed by 4D synchrotron X-ray nano-tomography* (European Synchrotron Radiation Facility User Meeting 2023. Grenoble, France. 06 Feb. 2023)

Ma, Y.; Raabe, D.: *Basic science behind green steel making* (2023 International Symposium on Hydrogen Metallurgy (ISHM2023). Chongli, China. 05 Sep. 2023)

Morgado F.F.; Bhatt, S.; Stephenson, L.; Mouton, I.; Neugebauer, J.; Raabe, D.; Freysoldt, C.; Gault, B.; Katnagallu, S.: *Role of simulations and experiments in analytical field ion microscopy* (Invited Seminar at University of Hyderabad, Hyderabad, India. 16 Feb. 2023)

Morgado F.F.; Bhatt, S.; Stephenson, L.; Mouton, I.; Neugebauer, J.; Raabe, D.; Freysoldt, C.; Gault, B.; Katnagallu, S.: *Experiment and Simulation Advances for atomic scale characterization using analytical field ion microscopy* (M&M 2023, Minneapolis, USA. 27 Jul. 2023).

Neugebauer, J.: *Current problems in Materials Sciences* (New Mathematics for the Exascale: Applications to Materials Science Tutorials. Los Angeles, CA, USA. 14 Mar. 2023)

Neugebauer, J.; Yang, J.; Todorova, M.; Hickel, T.: *Constructing Defect Phase Diagrams from Ab Initio Calculations and CALPHAD Concepts* (TMS Annual Meeting and Exhibition. San Diego, CA, USA. 19 Mar. 2023)

Neugebauer, J.; Körmann, F.; Hickel, T.: *Ab Initio Descriptors to Guide Materials Design in High-dimensional Chemical and Structural Configuration Spaces* (TMS Annual Meeting and Exhibition. San Diego, CA, USA. 21 Mar. 2023)

Neugebauer, J.; Poul, M.; Mathews, P.; Tehranchi, A.; Yang, J.; Todorova, M.; Hickel, T.: *Defect phase diagrams: Concepts, computational approaches and applications* (DPG Spring Meeting). Dresden, Germany. 26 Mar. 2023)

Neugebauer, J.: *Utilizing chemical complexity in electrochemistry* (Germany-Korea On-Site Plenary Discussion on Computational Electrochemistry at Korea University. Asan Science Building. Seoul, Korea. 17 Apr. 2023)

Neugebauer, J.; Yang, J.; Deißbeck, F.; Wippermann, S. M.; Todorova, M.: *Fully ab initio modeling of electrocatalytic and corrosion phenomena* (Korean Physical Society Meeting. Deajeon, Korea. 19 Apr. 2023)

Neugebauer, J.; Poul, M.; Mathews, P.; Tehranchi, A.; Yang, J.; Todorova, M.; Hickel, T.: *Construction and application of defect phase diagrams: Concepts and computational approaches* (Thermec 2023. Vienna, Austria. 02 Jul. 2023)

Neugebauer, J.; Deißbeck, F.; Surendralal, S.; Todorova, M.; Wippermann, S. M.: *Electrochemistry in a periodic supercell* (2023 "Computational Materials Chemistry" Telluride Workshop. Telluride, CO, USA. 17 Jul. 2023)

Neugebauer, J.: *Capturing the chemical complexity of HEAs by ab initio based modelling* (CHEAC Summer School 2023 - High Entropy Materials and their properties. Metaskolen-Jørlunde, Denmark. 15 Aug. 2023)

Neugebauer, J.: *Enabling next-generation materials science simulations by automated workflows* (NOMAD CoE Project Meeting, Aalto University. Espoo, Finland. 28 Aug. 2023)

Neugebauer, J.; Freysoldt, C.; Todorova, M.; Van de Walle, C. G.: *Charged defects in semiconductors and beyond* (32nd International Conference on Defects in Semiconductors. Rehoboth Beach, DE, USA. 10 Sep. 2023)

Neugebauer, J.: *Metastable defect phase diagrams as a road map for defect design* (Montanuniversität Leoben, Materials Science Colloquium. Leoben, Austria. 28 Sep. 2023)

Neugebauer, J.: *Boosting ab initio-based materials discovery by machine learning* (AI MSE 2023 - Artificial Intelligence in Materials Science and Engineering. Saarbrücken, Germany. 22 Nov. 2023)

Neugebauer, J.: *HPC based discovery and design of materials* (MPCDF Workshop "High-performance computing, artificial intelligence, and data-intensive applications in the Max-Planck Society." Schloss Ringberg, Tegernsee, Germany. 17 Dec. 2023)

Raabe, D.: *Green Steel Production by Hydrogen-Based Plasma Reduction of Iron Oxides* (2023 TMS Annual Meeting. San Diego, CA, USA. 20 Mar. 2023)

Raabe, D.: *The 2 Billion Ton Question—How Can Metals Become More Sustainable?* (Van Horn Distinguished Lecturer Series at Case Western Reserve University. Cleveland, OH, USA. 09 Oct. 2023)

Raabe, D.: *The Materials Behind Green Steel* (Van Horn Distinguished Lecturer Series at Case Western Reserve University. Cleveland, OH, USA. 10 Oct. 2023)



Raabe, D.: *The Interplay of Lattice Defects and Chemistry at Atomic Scale and Why it Matters for the Properties of Materials* (Van Horn Distinguished Lecturer Series at Case Western Reserve University. Cleveland, OH, USA. 11 Oct. 2023)

Raabe, D.: *The Materials Science Behind Hydrogen-Based Steel Making* (NIMS Award Commemorative Lecture 2023. Tsukuba, Japan. 06 Nov. 2023)

Raabe, D.: *Green Steel Production by Hydrogen-Based Plasma Reduction of Iron Oxides* (MRS Fall Meeting. Boston, MA, USA. 27 Nov. 2023)

Raabe, D.: *Accelerated Continuum Crystal Plasticity and Phase Field Microstructure Modeling Using U-Net* (MRS Fall Meeting. Boston, MA, USA. 01 Dec. 2023)

Ramachandramoorthy, R.: *Mechanical properties of additively manufactured copper microarchitectures under extreme loading conditions* (Department Seminar, Swiss Federal Laboratories for Materials Science and Technology. Dübendorf, Switzerland. 23 Jun. 2023)

Ramachandramoorthy, R.: *Additive micromanufacturing meets extreme micromechanics at constant strain rates* (RWTH Aachen, SFB 1394 Summer School. Aachen, Germany. 18 Sep. 2023)

Rao, Z.; Wei, Y.; Tung, P.-Y.; Xie, R.; Zhang, H.; Bauer, S.; Raabe, D.: *Machine learning-enabled high-entropy Invar alloy discovery* (Accelerated Discovery of new materials, 787 WE-Heraeus-Seminar. Physikzentrum Bad Honnef, Germany. 16 May 2023)

Rohwerder, M.: *Messung von Wasserstoffpermeation und -effusion mit der Kelvinsonde: Potentiometrie, Wasserstofftransport und -speicherung, Wasserstoffversprödung, Wasserstoffaufnahme und -abgabe* (3-Länder-Korrosionstagung. Frankfurt, Germany. 11 May 2023)

Rohwerder, M.: *Sustaining Tomorrow: The Crucial Role of Corrosion Science* (EUROCORR 2023, plenary talk. Frankfurt, Germany. 27 Aug. 2023)

Rohwerder, M.: *Probe Techniques for mapping effective local hydrogen activity and permeation rates* (International Hydrogen Conference (IHC) 2023. Park City, UT, USA. 17 Sep. 2023)

Rohwerder, M.: *Fundamental Aspects of Coating Delamination: Old Beliefs and New Insights* (GfKorr-Jahrestagung. Frankfurt a. Main, Germany. 07 Nov. 2023)

Roters, F.; Diehl, M.; Eisenlohr, P.; Shanthraj, P.: *DAMASK: The Düsseldorf Advanced Material Simulation Kit for studying multi-field crystal plasticity phenomena* (Seminar at Harbin Institute of Technology. Online. Shenzhen, China. 25 Jan. 2023)

Roters, F.; Hu, Y.; Diehl, M.: *Multi-Field Modelling of Crystal Plasticity and Damage* (CMCS 2023. Eindhoven, The Netherlands. 12 Oct. 2023)

Saksena, A.: *From Atoms to Functional Materials: Atom Probe Case Studies* (Talk at Malmö University. Malmö, Sweden. 23 Feb. 2023)

Saksena, A.; Sun, B.; Khanchandani, H.; Gault, B.: *Visualizing radiation-induced damage by Hydrogen/Deuterium* (DPG Spring Meeting 2023). Dresden, Germany. 29 Mar. 2023)

Scheu, C.: *Interfaces in renewable energy materials* (BIST Symposium on Microscopy, Barcelona, Spain. 10. Mar. 2023)

Scheu, C.; Zhang, S.: *Chemistry induced phase transition at $\Sigma 7$ grain boundary in Mg* (PICS 2023. Marseilles, France. 02 May 2023)

Scheu, C.: *Designing the functional properties of thermoelectric materials by grain boundary engineering* (Workshop on New Horizons in Materials Design, MPIE, Düsseldorf. 18 August 2023)

Scheu, C.: *New insights in energy materials by scale bridging characterization* (plenary talk) (Metallographie-Tagung, Leoben, Austria. 13 Sep. 2023)

Scheu, C.; Zhang, S.: *Hematite for light induced water splitting – improving efficiency by tuning distribution of Sn dopants at the atomic scale* (The International Symposium on Advanced Coatings for Energy – ISC4E 2023. Ben Guerir, Morocco. 27 Nov. 2023)

Stein, F.: *Fe–Al – An Exceptional Alloy System* (DGM Joint Meeting of the Technical Committee Intermetallic Phases (Fachausschuss Intermetallische Phasen (FA IP)) and Working Group Material Behavior at High Temperatures (Arbeitskreis Werkstoffverhalten bei hohen Temperaturen (AK HT)). Magdeburg, Germany. 15 May 2023)

Stein, F.; Distl, B.; Rashkova, B.: *High-temperature phase equilibria in the TiAl-based systems Ti–Al–Mo and Ti–Al–W* (Thermec'2023 – International Conference on Processing & Manufacturing of Advanced Materials. Vienna, Austria. 03 Jul. 2023)

Stein, F.: *Stability Competition between Laves Phase Polytypes* (IIT Hyderabad. Online. 01 Aug. 2023)

Stein, F.: *Alloying NdFeB – Constitution & Microstructure* (MSIT Advanced School – Seminar on Rare-Earth Materials & Magnet Technology. Stuttgart, Germany. 22 Nov. 2023)

Todorova, M.; Surendralal, S.; Deisenbeck, F.; Wippermann, S. M.; Neugebauer, J.: *The role of water at electrified solid/liquid interfaces under potential control* (Germany-Korea On-Site Plenary Discussion on Computational Electrochemistry at Korea University, Asan Science Building. Seoul, Korea. 17 Apr. 2023)

Todorova, M.; Yoo, S.-H.; Kim, S.-H.; Gault, B.; Neugebauer, J.: *Controlling doping of electrocatalysts through engineering impurities ... and the H/Pt/H₂O interface* (KPS 2023 Conference. Daejeon, Korea. 19 Apr. 2023)

Todorova, M.; Surendralal, S.; Deisenbeck, F.; Wippermann, S. M.; Neugebauer, J.: *Insights into Electrified Solid/Liquid Interfaces from Ab initio and Atomistic Molecular Dynamics Simulations* (CECAM – Young Research-

ers' School on Theory and Simulation in Electrochemical Conversion Processes. Paris, France. 22 May 2023)

Todorova, M.; Yoo, S.-H.; Kim, S.-H.; Gault, B.; Neugebauer, J.: *Controlling doping of electrocatalysts through engineering impurities* (2023 "Computational Materials Chemistry" Telluride Workshop. Telluride, CO, USA. 17 Jul. 2023)

Todorova, M.; Surendralal, S.; Wang, Z.; Deisenbeck, F.; Wippermann, S. M.; Neugebauer, J.: *Insights into processes at electro-chemical solid/liquid interfaces under potential control from first principles calculations* (34th IUPAP Conference on Computational Physics 2023 (CCP2023) (Keynote talk). Kobe, Japan. 04 Aug. 2023)

Todorova, M.; Surendralal, S.; Deisenbeck, F.; Wippermann, S. M.; Neugebauer, J.: *Insights into electrochemical solid/liquid interfaces under potential control from first principles and atomistic calculations* (TACO Colloquium, Universität Wien. Vienna, Austria. 23 Oct. 2023)

Vega Paredes, M.; Aymerich Armengol, R.; Scheu, C.: *Determining the degradation mechanisms and active species of electrocatalysts by identical location electron microscopy*. (NRF-DFG meeting "Electrodes for direct sea-water splitting and microstructure based stability analyses", Korean Institute for Energy Research. Jeju, South Korea. 18 Sept 2023)

Woods, E.; Aota, L. S.; Schwarz, T.; Kim, S.-H.; Douglas, J. O.; Singh, M. P.; Gault, B.: *In-situ cryogenic protective layers and metal coatings in cryogenic FIB* (IMC20 – 20th International Microscopy Congress - Pre-congress workshop, Cryogenic Atom Probe Tomography. Busan, South Korea. 09 Oct. 2023)

Zhang, S.: *Microstructure design in thermoelectric materials: Decoupling the transport properties and in situ observation at operation conditions* (Colloquium at Technische Universität. Darmstadt, Germany. 22 Feb. 2023)

Zhang, S.: *Microstructure design in thermoelectric materials: in situ observation of doping behavior and role of grain boundary phases* (Colloquium at RUB. Bochum, Germany. 10 Jul. 2023)

Zhang, S.; Kim, S.-H.; Mingers, A. M.; Gault, B.; Scheu, C.: *Operando Study on the corrosion of photo-electrocatalysts* (NRF-DFG meeting "Electrodes for direct sea-water splitting and microstructure based stability analyses", Kangwon National University. Chuncheon-si, South Korea. 08 Sep. 2023)

Zhang, S.; Kim, S.-H.; Mingers, A. M.; Gault, B.; Scheu, C.: *Operando Study on the activation of hydrogen evolution electrocatalysts* (NRF-DFG meeting "Electrodes for direct sea-water splitting and microstructure based stability analyses", Korean Institute for Energy Research. Daejeon, South Korea. 18 Sep. 2023)

Zhang, S.: *Electron microscopy: Resolution and imaging contrast* (DMG/DGK-AK9 Summer School "Advanced methods for the characterization of applied materials", MPI für Kohlenforschung. Mülheim (Ruhr), Germany. 26 Sep. 2023)

Zhou, X.; Ahmadian, A.; Hickel, T.; Gault, B.; Ophus, C.; Liebscher, C.; Dehm, G.; Raabe, D.: *Atomic Scale Analysis Reveals the Interplay between Grain Boundary Structure and Composition* (MRS 2023. Boston, MA, USA. 27 Nov. 2023)

Zhu, L.-F.: *Towards high throughput melting property calculations with ab initio accuracy aided by machine learning potential* (The third generation (3G) Calphad at KTH. Stockholm, Sweden. 06 Sep. 2023)

2024

Best, J. P.: *Relationships between local interface chemistry and mechanics probed through in situ micromechanical testing* (International Workshop on Materials Behavior at Micro- and Nano-Scale. Xi'an, China. 27 May 2024)

Bitzek, E.: *An atomistic Perspective on Fracture Toughness of inorganic Materials* (3rd FRASCAL Symposium. Erlangen, Germany. 08 Mar. 2024)

Bitzek, E.; Baranova, P.; Ghafarollahi, A.; Eggle-Sievers B.; Webler, R.; Gabel, S.; Neumeier, S.; Merle, B.; Göken M.; Patil, P.; Best J.: *Unveiling Microstructure Effects on Fracture: Atomistic Simulations, Mesoscale Models and Micromechanical Tests* (CIMTEC2024: materials in an explosively growing informatics world. Montecatini Terme, Italy. 20 Jun. 2024)

Bitzek, E.: *Veränderungsprozessen in Organisationen vs. Festkörpern: Plastische Verformung / Sprödbbruch* (AGD24 – Eine Veranstaltung für Düsseldorfer Unternehmer. Düsseldorf, Germany. 06 Sep. 2024)

Bitzek, E.: *Grain Boundaries: The Good, the Bad, and the Ugly* (Celebratory symposium for the birthday of Professor Mike Finnis, Department of Materials at Imperial College. London, UK. 12 Sep. 2024)

Bitzek, E.; Ghafarollahi, A.; Eggle-Sievers B.; Webler, R.; Gabel, S.; Neumeier, S.; Merle, B.; Göken M.; Patil, P.; Best J.: *Unraveling the Origins of Fracture Toughness by Integrating Micromechanical Testing and Atomistic Simulations* (Nanomechanical Testing in Materials Research and Development IX. Giardini Naxos, Italy. 06. Oct. 2024)

Bitzek, E.; *Atoms, Defects & Microstructure: Studying Mechanical Properties with Atomistic Simulations* (Workshop, SAFRAN Tec. Paris Saclay, France. 15 Oct. 2024)

Bitzek, E.: *Atoms, Defects & Microstructure: Investigating the Atomic-Scale Origins of Toughness and Strength* (Joint seminar of the Divisions of Energy and Materials, Dept. of Chemistry and Microstructure Physics, and the Dept of Physics, Chalmers University of Technology. Gothenburg, Sweden. 2024)

Brink, T.: *Defect phases and their line defects in fcc metal grain boundaries* (DPG Spring Meeting 2024. Berlin, Germany. 17 Mar. 2024)

Cheng, N.; Sun, H.; Pivak, Y.; Liebscher, C.: *In situ liquid phase 4D-STEM provides quantitative insights into the*



phase evolution of nanostructured Cu under electrochemical conditions (15th International Conference on Atomically Controlled Surfaces, Interfaces, and Nanostructures. Suzhou, China. 11 May 2024)

Dehm, G.; Devulapalli, V.; Schulz, F.; Soares Barreto, E.; Ellendt, N.; Jäggle, E. A.: *Strengthening of CoCrFe(Mn)Ni high entropy alloys by dislocation pinning: From Lattice friction & SRO to particle strengthening* (Possibilities and Limitations of Quantitative Materials Modeling and Characterization 2024. Bernkastel-kues, Germany. 26 May 2024)

Dehm, G.: *Atomic resolved imaging of grain boundary phase transitions in pure and alloyed metallic thin films* (17th International Conference on Intergranular and Interphase Boundaries in Materials (IIB 2024). Beijing, China. 08 Jul. 2024)

Dehm, G.: *Towards Understanding Dislocation Strengthening Mechanisms of Cr(Mn)FeCoNi high entropy alloys by advanced (S)TEM* (ELMINA 2024. Belgrade, Serbia. 09 Sep. 2024)

Dehm, G.: *Effects of Grain Boundary Structure and Chemistry on Plasticity in Metals* (Nanomechanical Testing in Materials Research and Development IX. Messina (Sicily), Italy. 06 Oct. 2024)

Dehm, G.: *TEM based characterization of defects in alloys* (Autumn School of Electron Microscopy 2024. Brno, Czech Republic. 17 Oct. 2024)

Dsouza, R.; Huber, L.; Swinburne, T. D.; Neugebauer, J.: *Sampling-free thermodynamics in bulk crystalline metals from the mean-field anharmonic bond model* (The 11th International Conference on Multiscale Materials Modeling. Prague, Czech Republic. 23 Sep. 2024)

Duarte, M.J.: *Micromechanical testing during hydrogen charging: examples on nanoindentation, pillar compression and nanoscratching* (Seminar talk at Tampere University. Tampere, Finland. 08 Feb. 2024).

Duarte, M.J.: *The role of hydrogen during mechanical testing* (Hydrogen analysis by APT Workshop. MPIE, Düsseldorf, Germany. 17 Apr. 2024).

Duarte, M.J.; Gopalan, H.; Rao, J.; Scheu, C.; Dehm, G.: *Micromechanics During Hydrogen Charging and the Study of Hydrogen Barrier Coatings* (International Conference on Metallurgical Coatings and Thin Films, ICMCTF 50. San Diego, CA, USA. 20 May 2024)

Duarte, M.J.; Rao, J.; Lee, S.; Gopalan, H.; Scheu, C.; Dehm, G.: *Micromechanics during hydrogen charging: the role of diffusible and trapped hydrogen* (Oxford - EPRI Workshop on Hydrogen Embrittlement. Oxford, UK. 25 Jun. 2024).

Elkot, M.; Sun, B.; Ponge, D.; Raabe, D.: *Strategizing for hydrogen embrittlement by protecting the weakest microstructural element* (ECF24 - European Conference on Fracture 2024 in Croatia. Zagreb, Croatia. 28 Aug. 2024)

Freysoldt, C.; Saxena, A.; Wang, N.; Sreekala, L.; Saikia, U.: *Perspectives for machine learning applied to data-rich*

experiments on complex materials (Colloquium Transregio 270 at Universität Duisburg-Essen. Duisburg, Germany. 12 Mar. 2024)

Freysoldt, C.; Saxena, A.; Wang, N.; Sreekala, L.; Saikia, U.; Gault, B.; Liebscher, C.: *Automated analysis of data-rich experiments for microstructure imaging* (Materials Science Engineering MSE 2022. Darmstadt, Germany. 24 -26 Sep. 2024)

Freysoldt, C.; Katnagallu, S.; Neugebauer, J.; Mishra, A.; Ashton, M. W.: *Perspectives for machine learning applied to data-rich experiments on complex materials* (Workshop on local probes of chemical bonding and atom probe tomography at RWTH Aachen, Germany. 12 Jun. 2024)

Hickel, T.; Grabowski, B.; Körmann, F.; Menon, S.: *Application of Density Functional Theory in the Context of Phase Diagram Modelling* (8th MSIT Winter School, Ringberg Castle, Tegernsee, Germany. 22 Jan. 2024)

Hickel, T.; Tehranchi, A.; Mathews, P.; Zendegani, A.; Zhang, S.; Scheu, C.; Neugebauer, J.: *Constructing defect phase diagrams from ab initio calculations* (Materials Science Workshop, Uppsala University, Sweden. 25 Apr. 2024)

Hickel, T.; Aydin, U.; Tehranchi, A.; Chakraborty, P.; Menon, S.; Janßen, J.; Neugebauer, J.: *Data driven research on hydrogen in metals* (DGM Fachausschuss "Wasserstoffeffekte in Werkstoffen", Saarbrücken, Germany. 06 May 2024)

Hickel, T.: *Research data infrastructures as enablers for materials design* (FLAIR Colloquium, CRC 1548, TU Darmstadt, Darmstadt, Germany. 10 Jun. 2024)

Hickel, T.; Tehranchi, A.; Chakraborty, P.; Freixes, M. L.; Zhao, H.; Gault, B.; Neugebauer, J.: *Fundamental insights into the mechanism of hydrogen embrittlement* (IC-MPPE; Integrated Comp. Materials, Process and Product Engineering, Leoben, Austria. 06 Jun. 2024)

Janssen, J.: *pyiron: workflows for the development and assessment of interatomic potentials* (Workshop "Machine Learning Force Fields at the Institute for Mathematical and Statistical Innovation (IMSI)". Chicago, IL, USA. 08 Apr. 2024)

Janssen, J.: *pyiron: Simulation Workflows for Data-Driven Materials Design* (Center for Nonlinear Studies (CNLS) Seminar, Los Alamos National Laboratory. Los Alamos, NM, USA. 29 Apr. 2024)

Janssen, J.: *Foundation Models for Materials Discovery* (Summer School at Center for Scientific Foundation Models. Michigan, MI, USA (online). 08 Jul. 2024)

Ma, Y.: *Hydrogen-based and Ammonia-based Direct Reduction of Iron Oxides* (Seminar at McMaster University. Online. 28 Feb. 2024)

Ma, Y.: *Basic science behind sustainable ironmaking with hydrogen and ammonia* (International Seminar on Hydrogen Use in Process Metallurgy. Trondheim, Norway. 15 May 2024)

Ma, Y.: *Hydrogen-based transformation of the steel industry* (Green Ironmaking with Hydrogen and Ammonia. Düsseldorf, Germany. 03 Jun. 2024)

Ma, Y.: *New insights into hierarchical microstructure formation during green ironmaking with hydrogen* (The ESRF ID03-ID11. Grenoble, France. 01 Aug. 2024)

Morgado F.F.; Bhatt, S.; Stephenso, L.; Mouton, I.; Neugebauer, J.; Raabe, D.; Freysoldt, C.; Gault, B.; Katnagallu, S.: *Advanced Data Processing and Ab Initio Simulations for Insights into Atom Probe Tomography Correlations, workshop on local probes of chemical bonding and atom probe tomography* (RWTH Aachen University, Germany. 12- 13 Jun. 2024)

Neugebauer, J.; Deisenbeck, F.; Wippermann, S. M.; Todorova, M.: *Discovery of Fundamental Reaction Mechanisms at Electrochemical Interfaces by Quantum Simulations* (63rd Sanibel Symposium. St. Augustine, FL, USA. 25 Feb. 2024)

Neugebauer, J.; Tehranchi, A.; Mathews, P.; Yang, J.; Todorova, M.; Hickel, T.: *Metastable Defect Phase Diagrams as a road map for defect design* (TMS Annual Meeting. Orlando, FL, USA. 03 Mar. 2024)

Neugebauer, J.; Tehranchi, A.; Mathews, P.; Yang, J.; Todorova, M.; Hickel, T.: *Metastable Defect Phase Diagrams as a road map for defect design* (FLAIR Colloquium talk, Technical University Darmstadt. Darmstadt, Germany. 25 Apr. 2024)

Neugebauer, J.; Menon, S.: *Maximizing High-Throughput Discovery and Machine Learning Efficiency Through Computational Workflows* (Machine Learning Modalities for Materials science. Ljubljana, Slovenia. 14 May 2024)

Neugebauer, J.; Deisenbeck, F.; Wippermann, S. M.; Todorova, M.: *Unveiling Fundamental Reaction Mechanisms at the Electrochemical Interface by Ab Initio Simulations* (245th ECS Meeting. San Francisco, CA, USA. 26 May 2024)

Neugebauer, J.; Deisenbeck, F.; Wippermann, S. M.; Todorova, M.: *Getting the Electrochemical Interface into an Ab Initio Supercell* (CECAM workshop "Electrochemical Interfaces in Energy Storage: Advances in Simulations, Methods and Models." Lausanne, Switzerland. 18 Jun. 2024)

Neugebauer, J.; Yang, J.; Wang, Z.; Wippermann, S. M.; Todorova, M.: *Challenges in developing machine learning potentials for fully explicit modeling of solid-liquid electrochemical interfaces* (CECAM Workshop "Machine Learning Potentials: From Interfaces to Solution" at RUB. Bochum, Germany. 27 Aug. 2024)

Neugebauer, J.: *Ab initio descriptors for materials design and discovery in high-dimensional chemical/structural space* (Celebratory symposium for the birthday of Professor Mike Finnis, Department of Materials at Imperial College London. London, UK. 12 Sep. 2024)

Neugebauer, J.; Körmann, F.; Ferrari, A.: *Navigating and exploiting the high-dimensional configuration spaces of*

high entropy alloys (The 11th International Conference on Multiscale Materials Modeling. Prague, Czech Republic. 22 Sep. 2024)

Neugebauer, J.: *AI and data driven design of sustainable materials* (KIT Materials Day. Karlsruhe, Germany. 16 Oct. 2024)

Raabe, D.: *Some Materials Science Aspects Behind Sustainable Steel* (Colloquium Lecture, Engineering Department, Freiburg University. Freiburg, Germany. 16 Jan. 2024)

Raabe, D.: *Basic Materials Science Aspects of Green Metal Production* (Royal Society Conference on Sustainable Metals: Science and Systems. London, UK. 06 Feb. 2024)

Raabe, D.: *The Two Billion Tonnes Question: How Can Research Help to Make Metals Sustainable?* (2024 TMS Annual Meeting. Orlando, FL, USA. 05 Mar. 2024)

Raabe, D.: *Atomic-Scale Perspective at Alloy-Design for Additive Manufacturing* (2024 TMS Annual Meeting. Orlando, FL, USA. 07 Mar. 2024)

Raabe, D.: *Transport and phase transformations phenomena in sustainable hydrogen-based steel production* (87th Spring Meeting of the German Physical Society. Berlin, Germany. 19 Mar. 2024)

Raabe, D.: *The Basic Science of Green Steel* (Colloquium Lecture, Physics Department, Augsburg University. Augsburg, Germany. 16 Jul. 2024)

Raabe, D.: *Sustainable Metals and Alloys* (Invited lecture, Berlin Brandenburg Academy of Sciences and Royal Society Symposium of Sustainable Chemistry. Berlin, Germany. 07 Oct. 2024)

Ramachandramoorthy, R.: *Nanoindentation and microcompression at constant high strain rates of upto 10⁵ s⁻¹* (3rd Materials Science Colloquium (68. Metallkunde Arlberg Kolloquium). Lech am Arlberg, Austria. 16 Apr. 2024)

Ramachandramoorthy, R.: *Physical Micrometallurgy Explorations: Microscale microstructure-architecture-extreme property relationships* (Nanomechanical Testing in Materials Research and Development IX. Messina (Sicily), Italy. 10 Oct. 2024)

Rao, Z.; Han, L.; Zhang, H.; Raabe, D.: *Active learning strategies for the sustainability of structural metals* (Royal Society Discussion Meeting on Sustainable Metals: Science and Systems. London, UK. 02 Jun. 2024)

Rohwerder, M.: *From Fundamental Mechanisms of Delamination to Self-Healing Coating Systems* (CorroZoom Webinar. Online. 19 Mar. 2024)

Rohwerder, M.: *Scanning Kelvin Probe Techniques for mapping effective local hydrogen activity and permeation rates at lateral high resolution and sensitivity* (188th ISIJ Meeting. Osaka, Japan. 18 Sep. 2024)

Roters, F.; Diehl, M.; Eisenlohr, P.: *Using DAMASK as material model in MSC Marc* (Marc Community Meeting. Online. 12 Jun. 2024)

Saxena, A.; Polin, N.; Kühbach, M.; Katnagallu, S.; Kontis, P.; Gault, B.; Freysoldt, C.: *A Machine Learning based Workflows to Quantify Atom Probe Tomography Data* (Workshop "Frontiers of APT Physics, Data Processing, Analysis and Reconstruction", Arlington, USA. 1-2 Aug. 2024)

Scheu, C.: *Spectroscopy* (Electron Microscopy Spring School 2024, Berlin, Germany. 05 Mar. 2024)

Scheu, C.: *Electron Energy-Loss Spectroscopy in a Scanning Transmission Electron Microscope: A versatile tool to study bonding characteristics in materials* (Atom Probe Tomography: A local probe of chemical bonds in solids? Aachen, Germany. 13 Jun. 2024)

Scheu, C.: *Insight in defects of energy materials: Aberration corrected STEM imaging coupled with 3D atom probe tomography* (Colloquium, Ludwig-Maximilians-Universität. München, Germany. 03 Jul. 2024)

Scheu, C.: *Unlocking the Stability of Ceramics in (Photo) Electro-Chemical Application and the Role of Defects* (Gordon Research Conference on Solid State Studies in Ceramics at the Mount Holyoke College. South Hadley, MA, USA. 08 Aug. 2024)

Scheu, C.; Bueno Villoro, R.; Abdellaoui, L.; Mattlat, D.; Jung, C.; Gault, B.; Zhang, S.: *New insights into thermoelectric materials through length-bridging characterization* (Workshop: Transverse Effects in Thermoelectrics Systems. Bonn, Germany. 14 Oct. 2024)

Schwarz, T.: *Introduction to (cryo)-atom probe tomography and its applications* (Belgium Physical Society meeting. Brussels, Belgium. 29 May 2024)

Stein, F.; He, Cuiyun: *Ternary Liquidus Surfaces and the Predictive Power of the Alkemade Theorem* (19th Discussion Meeting on the Thermodynamics of Alloys TOFA 2024. Lyon, France. 23 Sep. 2024)

Stein, F.; Distl, B.: *Phase Equilibria of TiAl-based Alloys Containing Ternary and Quaternary Additions of the Refractory Metals Nb, Mo, and W* (MRS Fall Meeting. Boston, MA, USA. 01 Dec. 2024)

Stratmann, M.: *Science Policy in a World of Dramatic Change* (GRC Aqueous Corrosion: Corrosion Challenges and Opportunities for the Energy Transition. New London, NH, USA. 07 Jul. 2024)

Todorova, M.; Surendralal, S.; Yang, J.; Neugebauer, J.: *Using ab initio calculations to unravel atomistic processes at electrified solid/liquid interfaces* (63rd Sanibel Symposium. St. Augustine, FL, USA. 28 Feb. 2024)

Todorova, M.; Surendralal, S.; Yang, J.; Deisenbeck, F.; Wippermann, S.; Neugebauer, J.: *Ab initio insights into atomistic processes at electrified solid/liquid interface* (DPG Spring Meeting, Berlin, Germany. 20 Mar. 2024)

Todorova, M.; Yoo, S.-H.; Yang, J.; Surendralal, S.; Deisenbeck, F.; Wippermann, S.; Neugebauer, J.: *First-principles modelling of electrified solid-liquid interfaces – from*

reaction mechanisms to synthesis (First-principles modeling and machine learning approaches in simulations of technologically relevant materials. Linköping, Sweden. 18 Apr. 2024)

Todorova, M.; Yang, J.; Surendralal, S.; Yoo, S.-H.; Deisenbeck, F.; Wippermann, S.; Neugebauer, J.: *Insights into atomistic processes at electrified solid/liquid interfaces from ab initio calculations* (245th ECS Meeting. San Francisco, CA, USA, 30 Mai 2024)

Todorova, M.: *Future directions in materials from modelling* (Future directions in materials research in Europe organised by the Materials Australia VIC-TAS Branch/ RMIT Europe. Online. 04 Jul. 2024)

Todorova, M.; Surendralal, S.; Deisenbeck, F.; Wippermann, S.; Neugebauer, J.: *Ab Initio Calculations for electrified solid/liquid interfaces – Challenges, insights and Opportunities* (GRC Aqueous Corrosion. New London, NH, USA. 10 Jul. 2024)

Todorova, M.; Yang, J.; Yoo, S.-H.; Surendralal, S.; Deisenbeck, F.; Wippermann, S.; Neugebauer, J.: *Insights into stability, reactivity and degradation of electrified solid/liquid interfaces from ab initio calculations* (Lorenz Workshop on "Multiscale modeling of electrochemical processes". Leiden, The Netherlands. 16 Aug. 2024)

Todorova, M.; Surendralal, S.; Yang, J.; Deisenbeck, F.; Wippermann, S.; Neugebauer, J.: *Advancing Electrochemical Insights: Ab Initio Control and Realistic Description of Solid-Liquid Interfaces* (75th ISE Annual Meeting. Montreal, CA, USA. 22 Aug. 2024)

Todorova, M.; Yang, J.; Surendralal, S.; Deisenbeck, F.; Wippermann, S.; Neugebauer, J.: *Using HPC workflows in modelling electrochemical solid/liquid interfaces* (NHR Conference 2024. Darmstadt, Germany. 09 Sep. 2024)

Todorova, M.; Surendralal, S.; Deisenbeck, F.; Wippermann, S.; Neugebauer, J.: *Atomic insights into fundamental processes at electrochemical solid/liquid interface by ab initio calculations* (38th Topical Meeting of the International Society of Electrochemistry: Nanomaterials in Electrochemistry. Manchester, UK. 10 Sep. 2024)

Todorova, M.: *Understanding fundamental processes at solid/liquid interfaces from first principles* (Celebratory symposium for the birthday of Professor Mike Finnis, Department of Materials at Imperial College London. London, UK. 12 Sep. 2024)

Todorova, M.; Yang, J.; Surendralal, S.; Deisenbeck, F.; Wippermann, S.; Neugebauer, J.: *Quantum mechanical based modelling of electrified solid/liquid interfaces – the example of corroding Mg* (11th International Conference on Multiscale Materials Modeling. Prague, Czech Republic. 25 Sep. 2024)

Zhang, S.: *Multivariate statistical analysis using Hyperspy* (Electron Microscopy Spring School, IRIS Adlershof, Berlin, Germany. 06 Mar. 2024)

Zhang, S.; Yu, Y.; Jung, C.; Mattlat, D. A.; Abdellaoui, L.; Scheu, C.: *In situ STEM observation of thermoelectric materials under heating and biasing conditions* (The 6th joint Sino-German workshop on advanced & correlative electron microscopy of catalysts, quantum phenomena & soft matter, Bad Honnef, Germany. 11 Jul. 2024)

Publications (as of 23 September 2024)

A comprehensive listing of scientific publications is available on the institute's web pages:

Computational Materials Design:
<https://www.mpi-susmat.de/2967008/publications>

Interface Chemistry and Surface Engineering:
https://www.mpi-susmat.de/2999511/Interface_Chemistry_and_Surface_Engineering

Microstructure Physics and Alloy Design:
<https://www.mpi-susmat.de/2987664/Publications>

Structure and Nano-/ Micromechanics of Materials:
<https://www.mpi-susmat.de/2999835/publications>

Nanoanalytics and Interfaces:
https://www.mpi-susmat.de/3118894/Nanoanalytics_and_Interfaces

Open Access:
<https://www.mpi-susmat.de/4263389/open-access-publications>

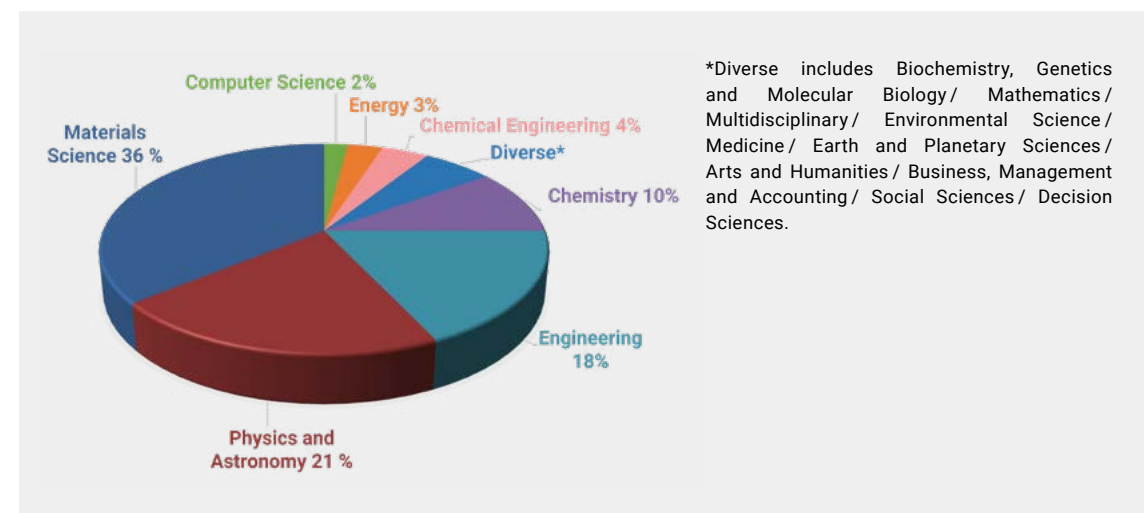
Publication statistics

The results of the fundamental scientific research conducted at MPI-SusMat are mainly published in peer-reviewed scientific journals. The following publication statistics are extracted from the Scopus database of indexed scientific journals.

From January 2022 to 23 September 2024, **693** peer-reviewed journal articles and reviews were published by the institute; over **60%** of the total set are **Open Access** and hence made broadly accessible across the scientific community but also to the general public, with a mix between Gold and Green as detailed below.

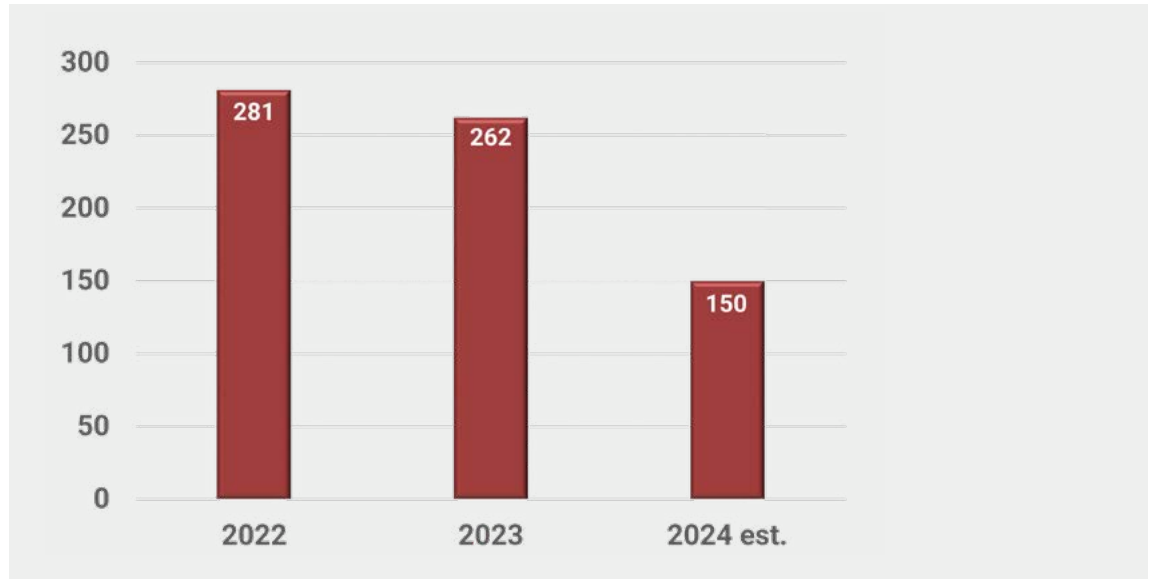
Publications by subject area

The set of publications between 2022 - 2024 from MPI-SusMat covers a broad range of topics, centred on materials science & engineering and physics, but also with forays into chemistry, energy and computer science.



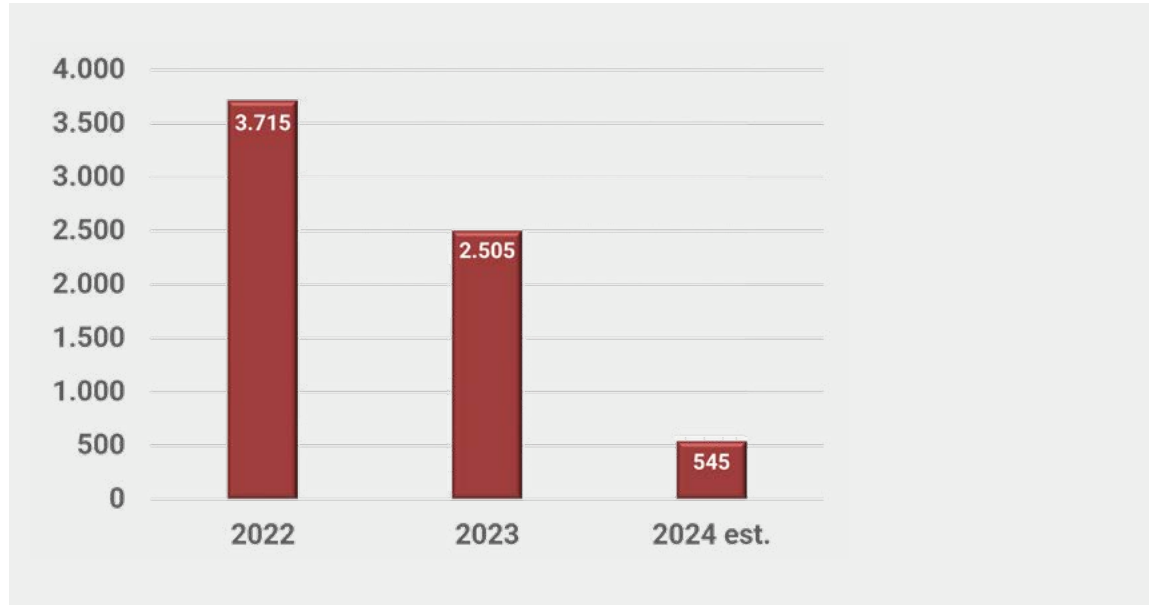
Scholarly output

A total of **693** publications have been released as of 23 September 2024.



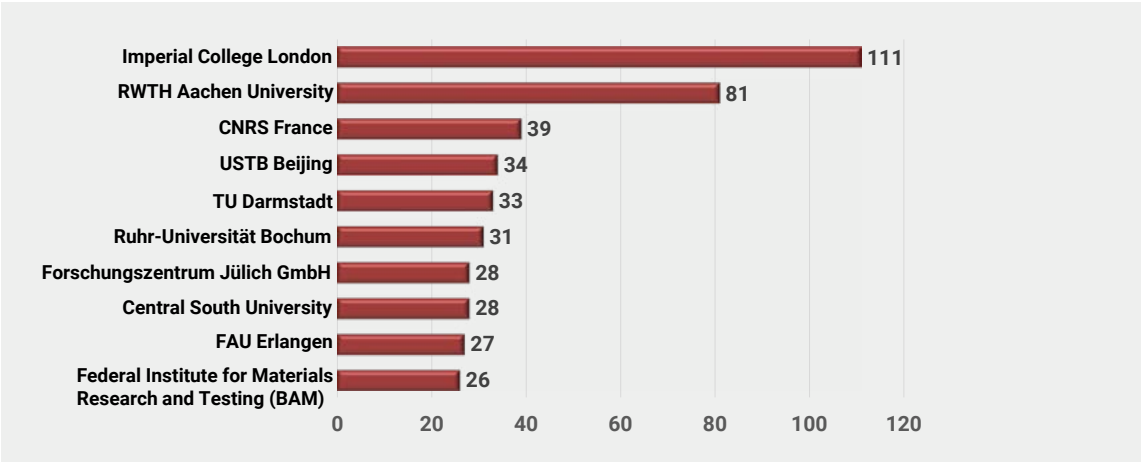
Citation count

A total of **6.765** citations were received by publications at the MPI-SusMat between January 2022 – September 2024 with an **average of 9.8** citations per publication.



This is the total number of citations for the publication set, with years being the years when articles were published, not the years in which citations were received.

Selected institutions participating in MPI-SusMat publications



Selected journals

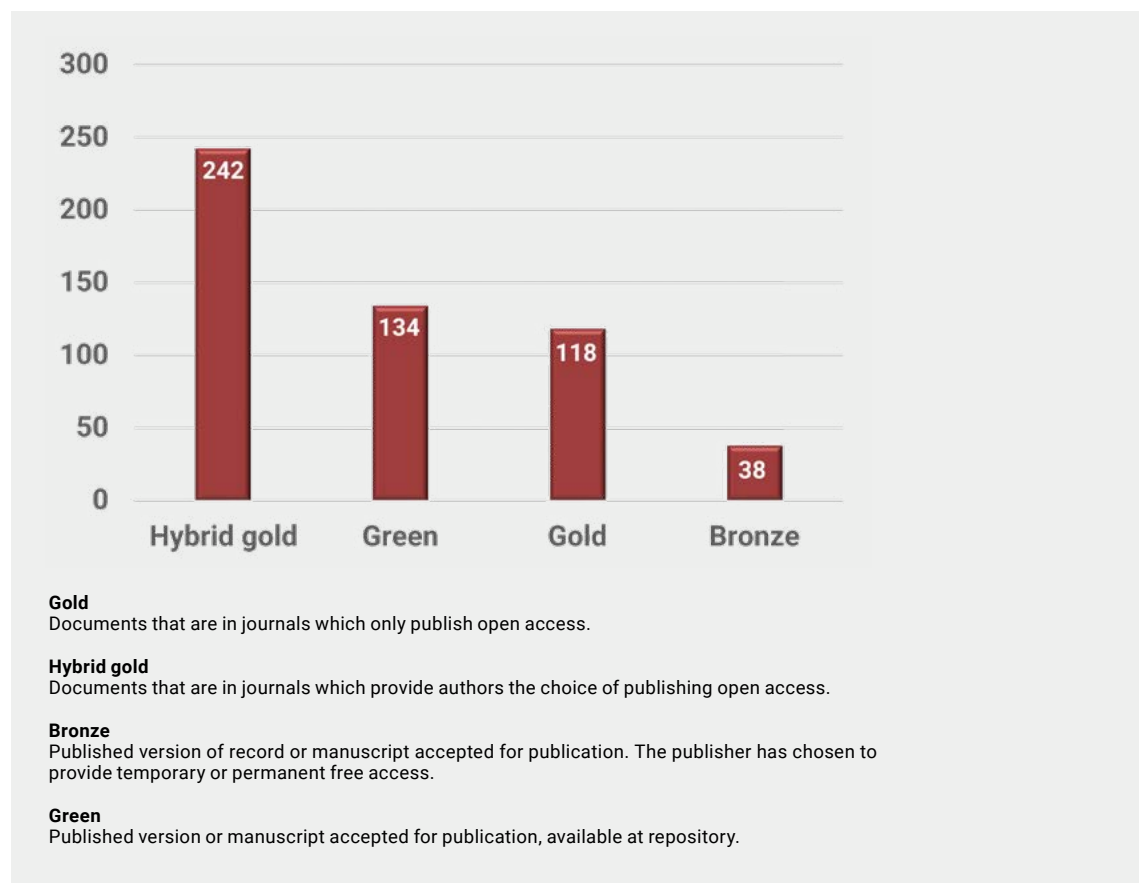
Name	Number of publications
Acta Materialia	81
Physical Review B (16), Physical Review Materials (14), Physical Review Applied (2), Physical Review Letters (2)	34
Scripta Materialia	33
Materials Science And Engineering A	27
Nature Communications	19
Materials and Design	19
Journal Of Alloys And Compounds	17
Nature	4
Nature Computational Science; Nature Materials; Nature Reviews Materials (2 each)	6
Science	2

Open access

A total of **448** papers were published open access between 2022 and 23 September 2024.

A list of our open access publications is available on our webpage:

<https://www.mpi-susmat.de/4263389/open-access-publications>



Habilitation, doctoral, master and bachelor theses

Doctoral theses

2021 (not included in Scientific Report 2019 - 2021)

Dr.-Ing. T.S. Prithiv: Grain boundary segregation of boron and carbon and their local chemical effects on the phase transformations in steels (RWTH Aachen)

2022

Dr.-Ing. A. Ahmadian: Atomic-scale characterisation of grain boundary structure and segregation in bcc-iron (Ruhr-Universität Bochum)

Dr. rer. nat. M. Alam: Development and application of semi-empirical interatomic potentials to study interface faceting and fracture (Universität Paderborn)

Dr.-Ing. L.-M. Baumgartner: Klärung polymerer Anbindungsmechanismen und Untersuchungen Stahloberflächen (Ruhr-Universität Bochum)

Dr. rer. nat. R. Changizi: Structural Analysis and Correlative Cathodoluminescence Investigations of Pr (doped) Niobates (RWTH Aachen), **with distinction "summa cum laude"**

Dr.-Ing. V. Devulapalli: Microstructure and grain boundary evolution in titanium thin films (Ruhr-Universität Bochum)

Dr.-Ing. B. Distl: Phase equilibria and phase transformations of Ti-Al-X (X=Nb, Mo, W) alloys for high-temperature structural applications between 700 and 1300 °C (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

Dr. rer. nat. L. Gomell: Advancing the understanding of the microstructure-property relationship in non-toxic and cost-effective thermoelectric Heusler compounds (RWTH Aachen)

Dr.-Ing. L. Han: Designing strong and ductile soft-magnetic multicomponent alloys (RWTH Aachen), **with distinction "summa cum laude"**

Dr. rer. nat. O. Hegde: Ab initio based study of magneto-chemo-structural coupling in complex alloys (Universität Duisburg-Essen)

Dr.-Ing. H. Khanchandani: Investigation of hydrogen embrittlement in a high manganese twinning induced plasticity steel: a correlative electron microscopy and atom probe tomography study (RWTH Aachen)

Dr.-Ing. T. Oellers: Development of combinatorial methods to tailor electrical and mechanical properties of Cu-based thin-film structures (Ruhr-Universität Bochum)

Dr.-Ing. J. M. Prabhakar: Fundamental investigation of the cathodic delamination behaviour of model polymer coating on novel chromium-based coatings electrodeposited from a trivalent chromium-formate electrolyte (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

Dr.-Ing. V. Shah: Full-field simulations of dynamic and meta-dynamic recrystallization (RWTH Aachen)

Dr. rer. nat. L. Sreekala: Ab-initio study on the correlation between phase stabilities and interstitial solubilities in chemically complex carbides (Ruhr-Universität Bochum)

Dr.-Ing. K. Srikakulapu: Critical factors for bearing failures by localized severe plastic deformation (RWTH Aachen)

Dr.-Ing. H. Tsybenko: On the cementite behavior during tribology and experimental methods of microscale wear (Ruhr-Universität Bochum)

Dr.-Ing. C. Yilmaz: Influence of Processing Parameters, Crystallography and Chemistry of Defects on the Microstructure and Texture Evolution in Grain-Oriented Electrical Steels (RWTH Aachen)

Dr.-Ing. Y. Yin: Self-heating coatings based on conducting polymer for intelligent corrosion protection (Ruhr-Universität Bochum)

2023

Dr.-Ing. S. Ahmad: Fundamental investigation of the atomic structures of [111] tilt grain boundaries, their defects and segregation behaviour in pure and alloyed Al (Ruhr-Universität Bochum)

Dr.-Ing. A. Atila: Influence of Structure and Topology on the Deformation Behavior and Fracture of Oxide Glasses (Friedrich-Alexander-Universität Erlangen-Nürnberg)

Dr.-Ing. R. Aymerich Armengol: Synthesis, Structure, and Stability of 2D Nanostructured Oxides and Chalcogenides (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

Dr.-Ing. R. Bueno-Villoro: Effect of grain boundary phases in the thermoelectric properties of half Heusler materials (Ruhr-Universität Bochum)

Dr.-Ing. F. J. Gallardo Basile: Crystal Plasticity Modeling of Bainite Dual-Phase Steels (RWTH Aachen)

Dr.-Ing. A. Gedsun: Fe-Al-Nb(-B) alloy development for structural applications at high temperatures (Ruhr-Universität Bochum)

Dr.-Ing. R. Hosseinabadi: Dislocation transmission through coherent and incoherent twin boundaries in copper at the micron scale (Ruhr-Universität Bochum)



Dr.-Ing. R. M. Jentner: Phase identification and micromechanical characterization of an advanced high-strength low-alloy steel (Ruhr-Universität Bochum)

Dr.-Ing. Z. Kahrobaee: Critical assessment and investigation of the Ti–Al–X (X = Si, Zr, O) systems (Ruhr-Universität Bochum)

Dr.-Ing. C. Kasdorf Giesbrecht: Electrochemistry of "dry" metal surfaces with regard to atmospheric corrosion (Ruhr-Universität Bochum)

Dr.-Ing. N. Khayatan: Investigation of Key Parameters in Cathodic Delamination of Organic Coatings and Quantification of their Role (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

Dr.-Ing. L. P. Langenohl: Atomic scale observations of grain boundary phase transformations and segregation effects in copper (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

Dr.-Ing. M. López Freixes: Nanoscale mechanisms of stress-corrosion cracking of 7xxx Al-alloys, (RWTH Aachen) **with distinction "summa cum laude"**

Dr.-Ing. P. P. Patil: Influence of plastic anisotropy on the deformation behaviour of Austenitic stainless-steel during single micro-asperity wear (Ruhr-Universität Bochum)

Dr.-Ing. J. Rao: Hydrogen effects on the mechanical behaviour of FeCr alloys investigated by in-situ nanoindentation (Ruhr-Universität Bochum)

Dr.-Ing. S. Roongta: Development of an Integrated Computational Materials Engineering Tool to Perform Multi-Physics Simulations at the Grain Scale (RWTH Aachen)

2024

Dr.-Ing. X. Dong: Hydrogen Associated Decohesion and Localized Plasticity in a Dual-phase Lightweight Steel (RWTH Aachen)

Dr.-Ing. M. N. Elkot: Hydrogen embrittlement in austenitic high manganese lightweight steel: Effect of k-carbides precipitation and boron doping (RWTH Aachen)

Dr.-Ing. A. Ganapathi: The hydrogen electrode in the "dry": on the effect of electrode material and relative humidity (Ruhr-Universität Bochum)

A. Jena: Calculating Indentation Schmid Factor (ISF) and Analyzing Complex Stress State During Nanoindentation Using Crystal Plasticity Finite Element Simulation (Ruhr-Universität Bochum)

Dr. rer. nat. F. F. Morgado de Oliveira: Enabling true atomic-scale analytical imaging, application to solute segregation at crystal defects in high-temperature materials (Ruhr-Universität Bochum)

Dr.-Ing. M. C. Paolantonio: Doping Effects on Interfaces, Phases and Properties of Al (Ruhr-Universität Bochum)

Dr.-Ing. A. Saxena: Machine learning workflows for automatic analysis of atom probe tomography data (RWTH Aachen)

Dr.-Ing. T.M. Schwarz: Application of cryo-atom probe tomography to the study of liquid - solid interfaces at near atomic scale, (RWTH Aachen) **with distinction "summa cum laude"**

Master theses

2023

W. Mohammed: Investigation of Fe Impurity Tolerance in Recycled Al-Si Alloys (RWTH Aachen)

N. Nicolin: Synthesis and Characterization of Reactive Magnetron Sputtered Fe_{1-x}O Thin Films (Heinrich-Heine-Universität Düsseldorf)

Y.-F. Wang: Porosity evolution during hydrogen-based direct reduction of hematite probed by 4D synchrotron X-ray nanotomography (RWTH Aachen)

2024

K. Hemke: Influence of Manganese Oxides on the Hydrogen-based Direct Reduction of Hematite Pellets (Hochschule Bonn-Rhein-Sieg)

S. Shankar: Thermodynamic-guided sustainable multicomponent alloy design via hydrogen-based direct reduction (RWTH Aachen)

Bachelor theses

2023

C. Mehrmann: Studying the Molecular and Nanostructure of Supported Ionic Liquid Phases on Silicon (Hochschule Niederrhein)

A. Vishwakarma: Impact of defect structures on Hydrogen diffusion in Nickel, Materials Science and Simulation (Ruhr-Universität Bochum)

J.M. Währisch: Legierungsdesign von Pulver auf Eisenbasis als Metallbrennstoff: Die Rolle von Legierungselementen (Hochschule Düsseldorf)

2024

Sihan Zhang: Surface Enhanced Spectroscopy Investigation of Ni-based Oxygen Evolution Reaction catalysts (Nankai University, Tianjin, China)

Scientific community service activities of the directors

Prof. Gerhard Dehm

Member of the Selection Committee for Applicants for Max-Planck-Lise-Meitner Groups (since 2018)

Member of the Selection Committee for the Allocation of Humboldt Research Fellowships (since 2017)

Member of the Selection Committee for Applicants for Max-Planck-Research Groups (since 2014)

Member of the board of trustees (Kuratorium) of the KSB Stiftung (since 2016)

Member of the Board of Governors of Acta Materialia Inc. (since 2013)

Editorial Board of Advanced Engineering Materials (Wiley) (since 2013)

Member of the Editorial Board International Journal of Materials Research (Hanser) (since of 2007)

Member of the Editorial Board Berg- und Hüttenmanische Monatshefte (Springer) (since of 2009)

Prof. Jörg Neugebauer

Director of the Advanced Study Group "Modelling" (2008 - 2024) at the International Centre of Advanced Materials Simulation ICAMS and ICAMS Fellow (since 2024)

Member of the "Fixed-term W2 appointment committee" of the Max Planck Society (since 2023)

Member of the NHR (National High-performance Computing) 2023 Conference Board

Speaker (since 2022) of the International Max Planck Research School for Sustainable Metallurgy - from Fundamentals to Engineering Materials (IMPRS-SusMet) at the Max Planck Institute for Sustainable Materials, the Ruhr-Universität Bochum, the University of Duisburg-Essen and the Max-Planck-Institut für Kohlenforschung

Member of the NFDI-MatWerk-Consortium (since 2021)

Elected member of the working group Metals and Materials (AGMM) of the German Physical Society (DPG) (since 2019)

Member of the Management Board of the Consortium Material Digital (since 2019)

Member of the Supervisory Board (Aufsichtsrat) of the Karlsruhe Institute of Technology (KIT) (since 2019)

Member of the scientific committee of the "Models and Data for Plasma-Material Interaction in Fusion Devices (MoD-PMI)" workshop series (since 2016)

Chair of the expert committee "Digital transformation in materials engineering" of the Association of German Engineers (VDI) (since 2016)

Member of the HLRB (supercomputer in Bavaria) steering committee of the Leibniz computer centre of the Bavarian Academy of Sciences (since 2012)

Elected Member of the Academy of Sciences and Art in North Rhine-Westphalia (since 2010)

Member of the Psi-k scientific steering committee and speaker of the working group *Structural materials (including metallic alloys, minerals, amorphous solids and materials under extreme conditions)*, previously *Applications to real materials: Structural materials* (since 2009)

Member of the IT-advisory board (BAR) of the Max Planck Society (since 2006)

Member (since 2004) and speaker (2014 - 2022) of the International Max Planck Research School for Interface Controlled Materials for Energy Conversion (IMPRS-SurMat) at the Max-Planck-Institut für Eisenforschung, the Ruhr-Universität Bochum, the University of Duisburg-Essen, the Max-Planck-Institut für Kohlenforschung and the Max Planck Institute for Chemical Energy Conversion

Member of the Foundation Board of the Heinz-Billing-Prize for the advancement of scientific computation (since 2019)

Prof. Dierk Raabe

Member of the Selection Board of the scholarship programme of the Alexander von Humboldt Foundation (since 2007)

Member of selection board of the Alexander von Humboldt Professorship programme (since 2017)

Member of the Governors Board of Acta Materialia Inc. (2007-2015)

Chairman of the RWTH Board of Governors (Hochschulrat der RWTH Aachen) (2012-2017)

Member of the Council of Science and Humanities of the German Government (Wissenschaftsrat) (2010 - 2016)

Senator of the Helmholtz Association for the Research Field Key Technologies (since 2017)

Member Northrhine-Westfalian Academy of Sciences (since 2008)

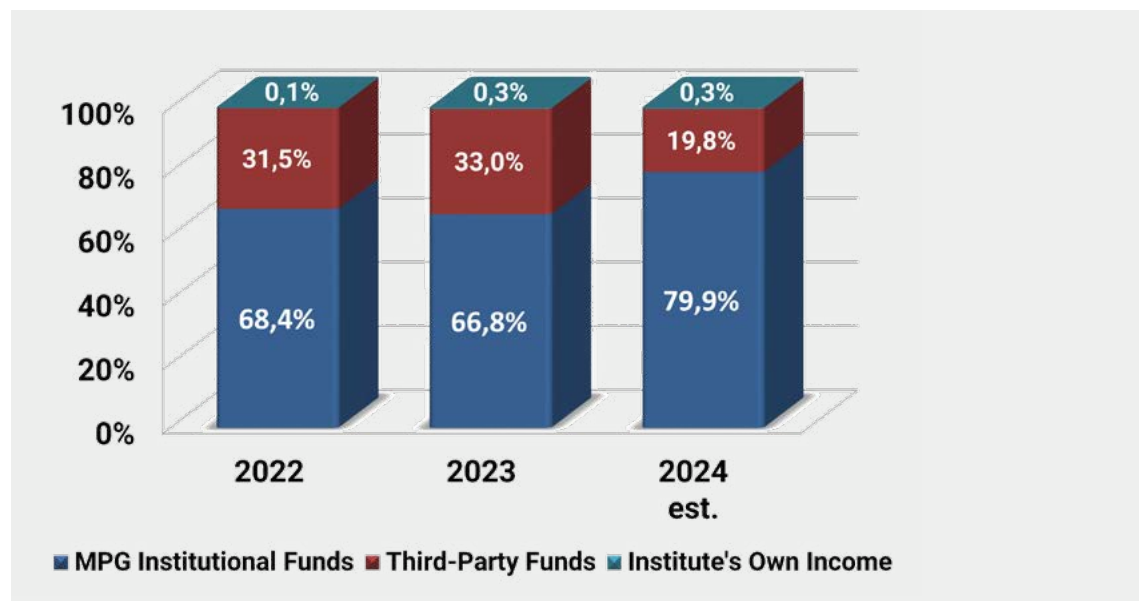
Member National Academy Leopoldina (since 2013)

Honorary Professor at Katholieke Universiteit Leuven, Belgium (since 2014)

Budget of the institute

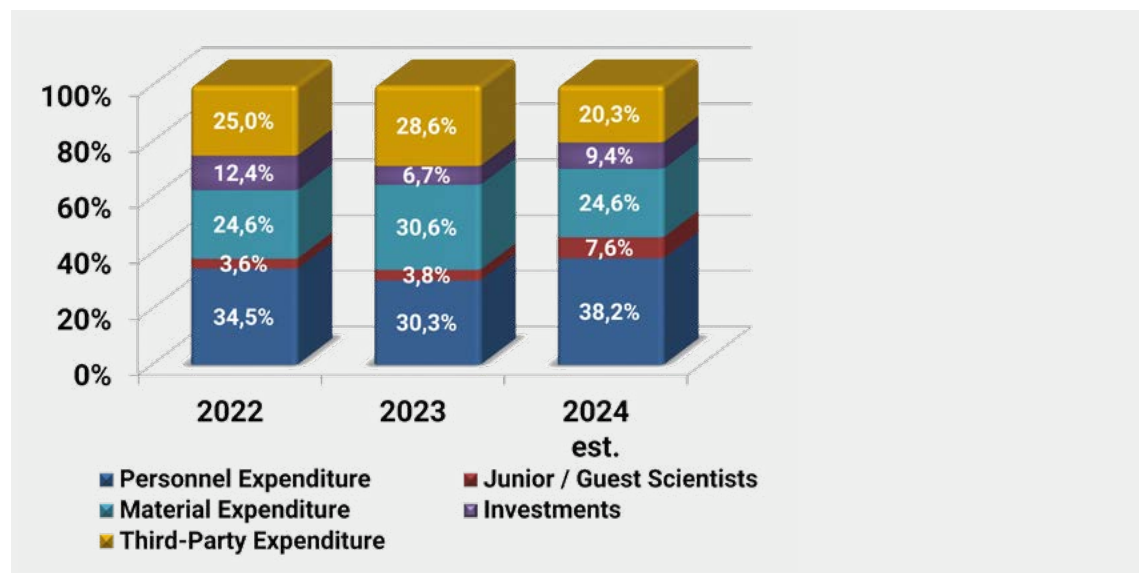
Revenue

(Percentual contributions to total revenue without appointment-related investment funds and general reconstruction of the buildings; year 2024 data estimated)



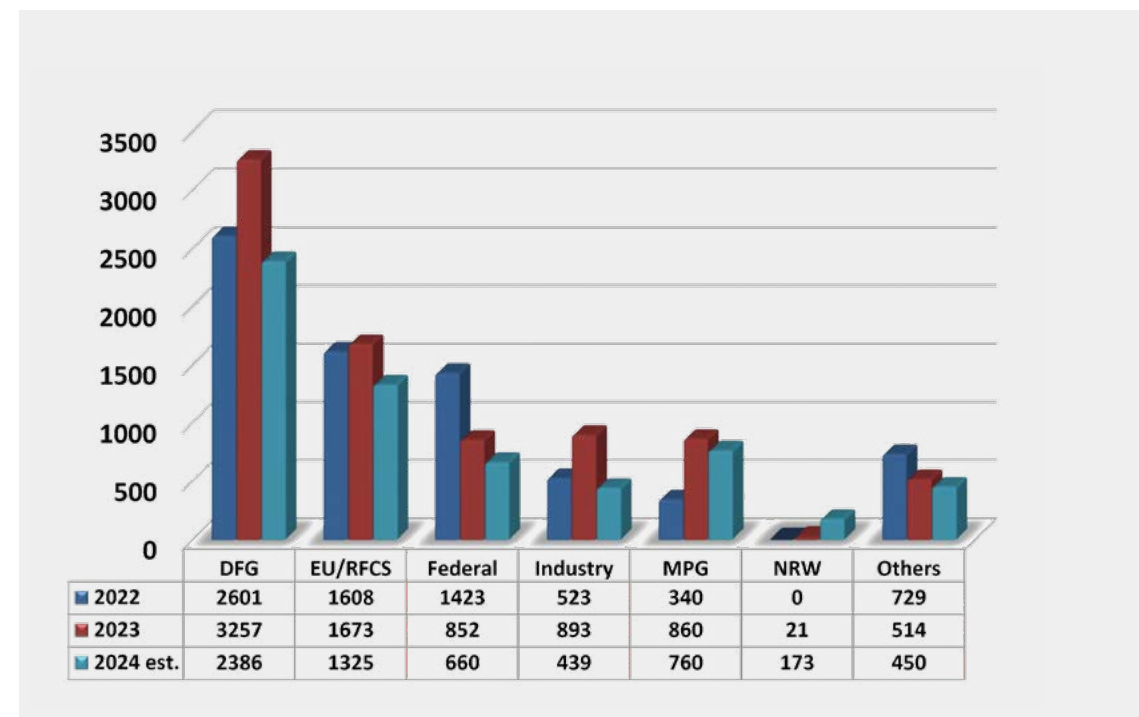
Expenditure

(Percentual distribution of total expenditure; investments include large-scale apparatus, electronic data processing, appointment-related investments, separate investment for basic equipment; year 2024 data estimated)



Third-party funds

(Contributions in 1,000 € to total revenue including personnel, material and investments, year 2024 data estimated)



DFG: German Science Foundation

EU: European Union

RFCS: Research Fund for Coal and Steel

Federal: BMBF & BMWK

BMBF: Federal Ministry of Science and Education

BMWK: Federal Ministry for Economic Affairs and Climate Action Industry incl. Christian Doppler Society and MaxNet

MPG: Max Planck Society

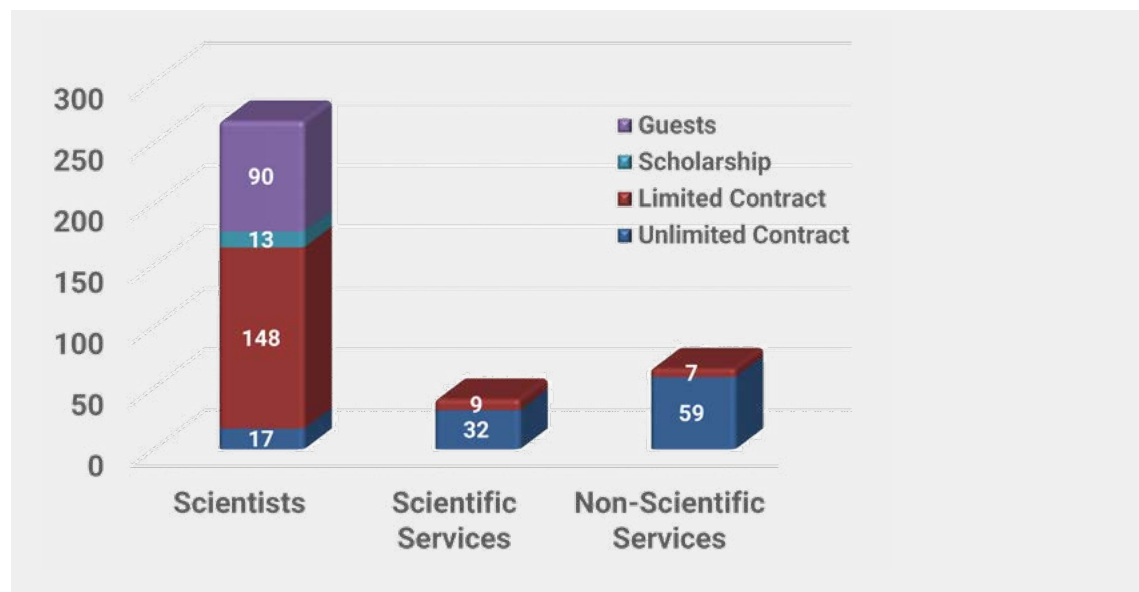
NRW: State of North Rhine-Westphalia

Others: Diverse revenue on material costs (e.g. Humboldt Foundation, Merkle Foundation)

Personnel structure

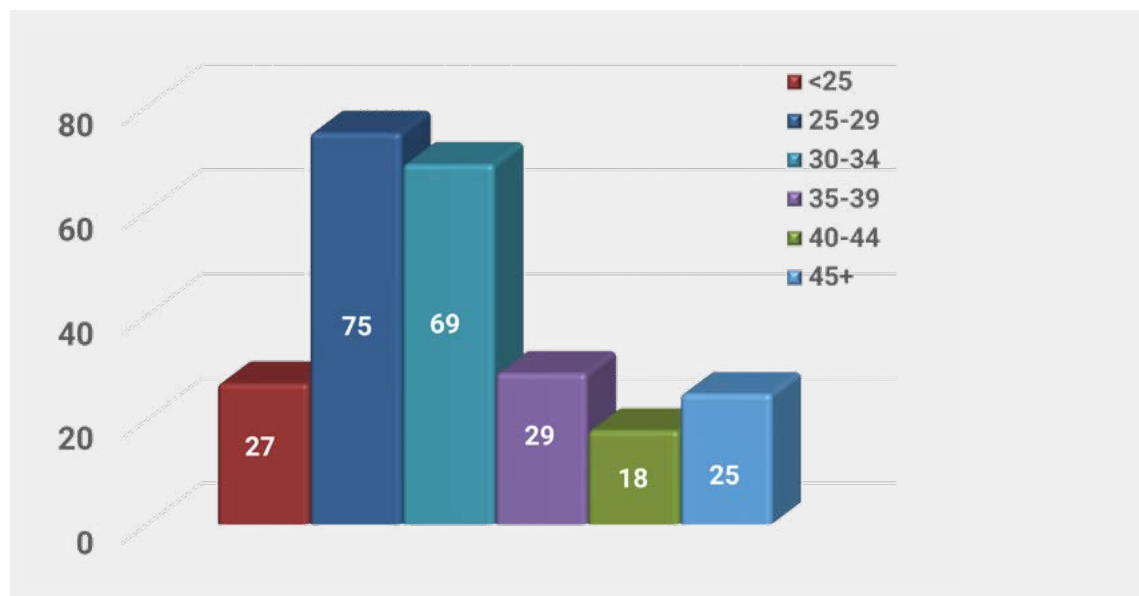
Number of occupied scientific / non-scientific positions

(Absolute numbers, August 2024)



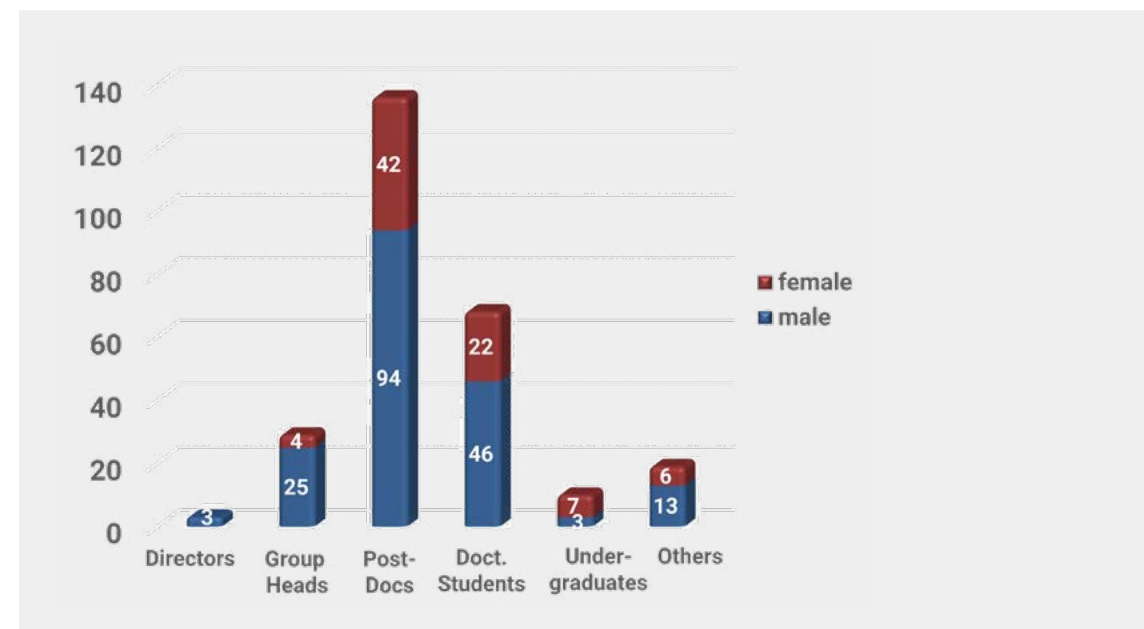
Age distribution of scientists

(Absolute numbers, August 2024)



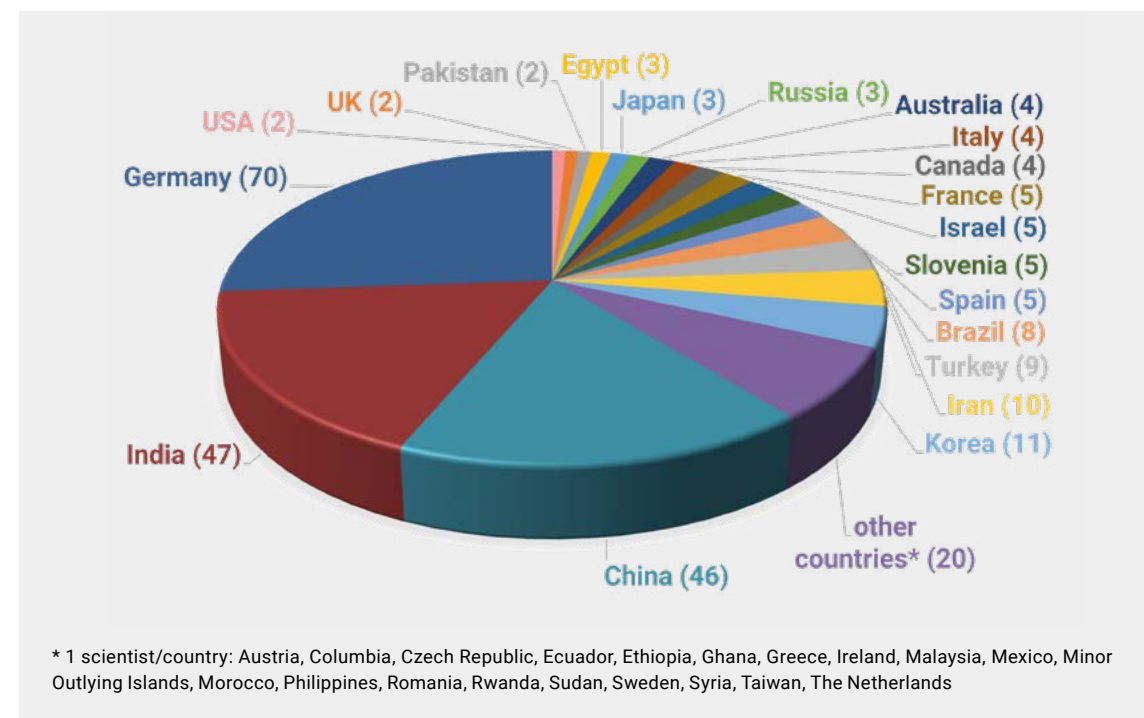
Gender distribution of scientists

(Absolute numbers, August 2024)



Scientists and their home countries

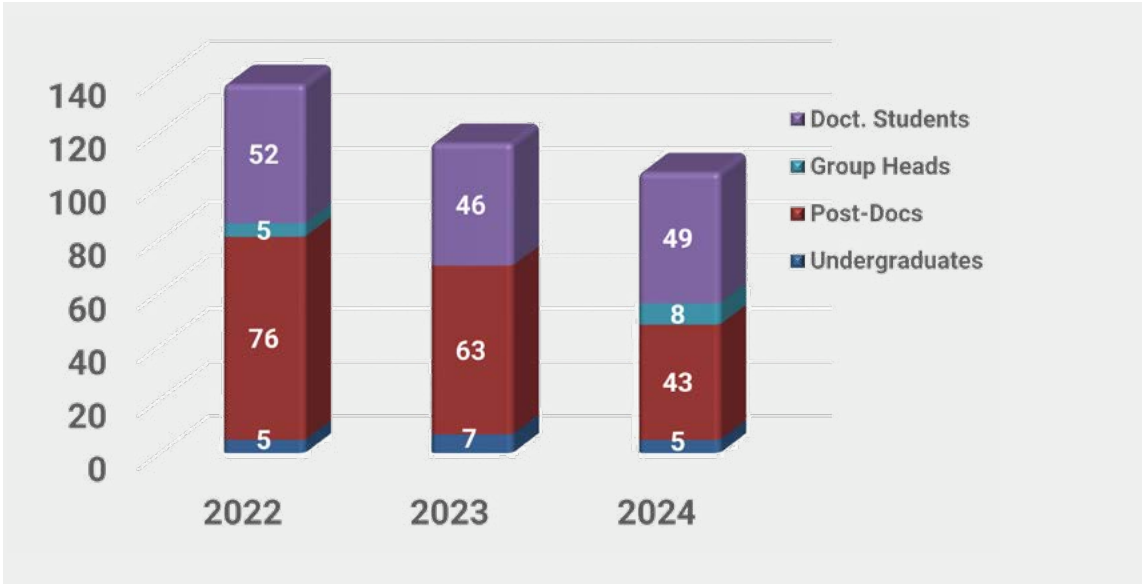
(Absolute numbers, August 2024)



Number of junior scientists

(Absolute numbers, year 2024 data estimated)

Financed via third-party funds



Not financed via third-party funds

