



Part IV.

General information and statistics

Boards, directors, Max Planck fellows, and external scientific members	228
Guest scientists	230
Scientific honours & appointments	233
Participation in research programmes	237
Collaboration with national and international universities and research institutes	242
Collaborating industrial partners and patents	245
Conferences, symposia and meetings organized by the institute	247
Institute colloquia and invited seminar talks	249
Lectures and teaching at university	254
Invited talks at conferences and colloquia	256
Publications	269
Habilitation, doctoral, master and bachelor theses	275
Scientific community service activities of the directors	278
Budget of the institute	279
Personnel structure	281



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

Supervisory board (as of January 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

Martin BAUES
Saarstahl AG, Völklingen, 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 GÜNNEWIG
Ministry of Culture and Science of the State of North
Rhine-Westphalia, Düsseldorf, Germany

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

Prof. Dr. Axel SCHÖLMERICH
Rector, Ruhr-Universität Bochum, Bochum, Germany

Scientific advisory board (as of January 2022)

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

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

Prof. Dr. Peter GUMBSCHE
Fraunhofer-Institut für Werkstoffmechanik (IWM),
Freiburg, Germany

Prof. Dr. Wolfgang JÄGER
Kiel University, Christian-Albrechts-Universität (CAU) zu
Kiel, Kiel, Germany

Prof. Dr. Michael John MILLS
Ohio State University, Columbus, USA

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

Dr. André SCHNEIDER
Vallourec Deutschland GmbH, Düsseldorf, Germany

Prof. Dr. Christopher A. SCHUH
Massachusetts Institute of Technology (MIT), Cam-
bridge, USA

Prof. Dr. Herman TERRYN
Vrije Universiteit Brussel (VUB), Brüssel, Belgium

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)**

Prof. Dr. rer. nat. Martin STRATMANN (since Jan. 2000 /
on leave for the time of his presidency of the MPG)

*Provisional Head of the Department Interface Chemistry
and Surface Engineering

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

Max Planck fellows:

Prof. Dr. Jochen M. SCHNEIDER, Ph.D., RWTH Aachen
University (Oct. 2015 - Sept. 2020)

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

External scientific members:

Prof. Dr. Mats HILLERT, Stockholm, Sweden

Prof. Dr. Reiner KIRCHHEIM, Göttingen



Guest scientists

Between January 2019 and November 2021 the Max-Planck-Institut für Eisenforschung GmbH hosted in total **158** international guest scientists.

Alexander von Humboldt Foundation

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

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

In November 2021 the following Humboldt fellows were awarded who will join the MPIE in 2022:

- **4** Humboldt Research Fellowships for Postdoctoral Researchers
- **1** Humboldt Research Award

Also in November 2021, B. Gault and D. Raabe became **Humboldt scouts in frame of 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 will be granted directly.

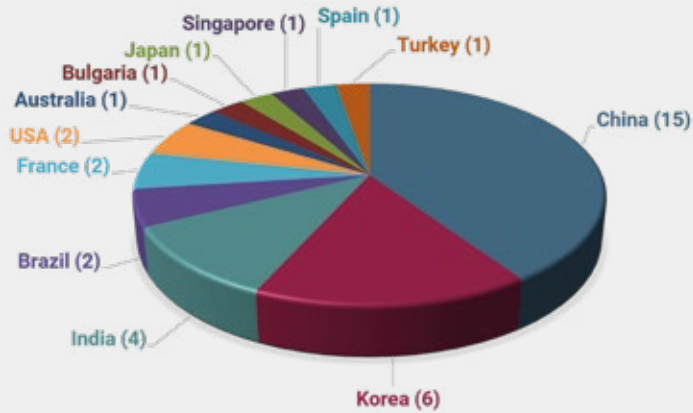
In the ranking of the Humboldt Foundation, the institute **was ranked first in Engineering Sciences** in 2020. It was also **ranked 3rd place over all sciences** of non-university research institutions.

Engineering Sciences

Absolute rankings	Institutions	Number of guest researchers per institution				Total number
		Fellows		Award winners		
		female	male	female	male	
1	MPI für Eisenforschung GmbH, Düsseldorf	5	25	3		33
2	MPI für Intelligente Systeme, Stuttgart		12	1	3	16
3	Forschungszentrum Jülich (FZJ)	4	7		1	12

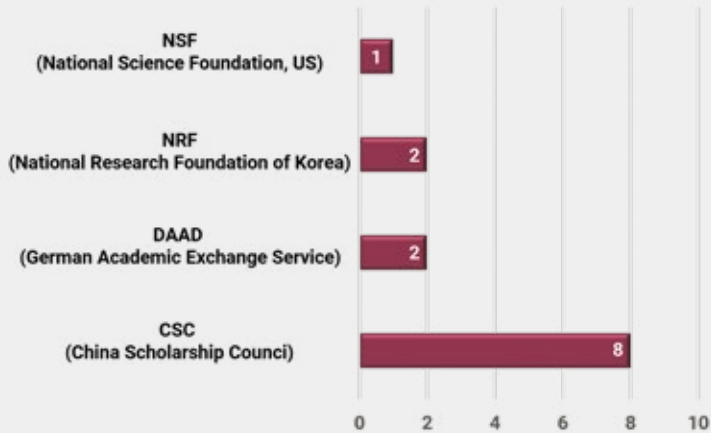
Source: <https://www.humboldt-foundation.de/en/explore/figures-and-statistics/humboldt-rankings#c18797>

Home countries of guests from the Alexander von Humboldt Foundation



Diverse fellowships

13 scientists came to the MPIE with diverse fellowships:

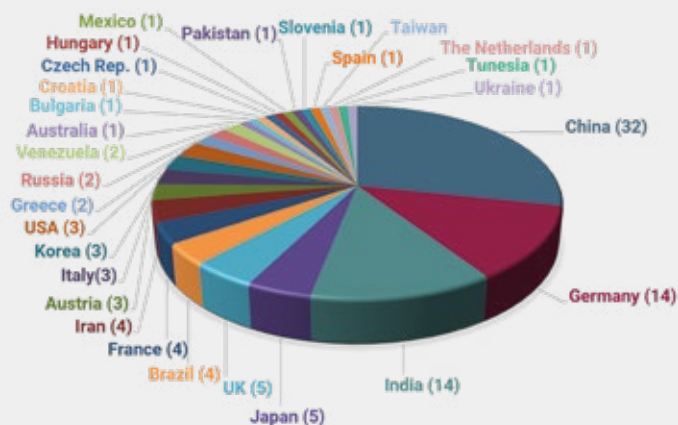




International research cooperation

With **113** scientists, the majority of our guest scientists stayed with us in frame of research cooperations. **27** of them being MPIE alumni.

Number of guest scientists per country



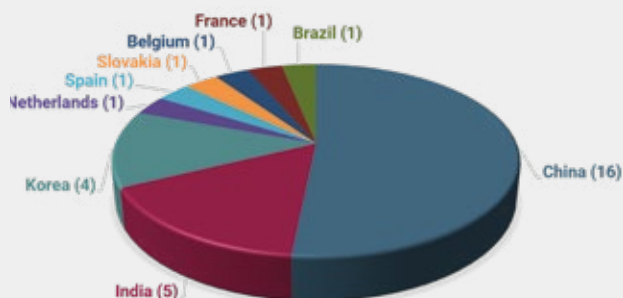
A detailed list of our “National and International Cooperation Partners” can be found from page 242 onwards.

MPIE guest programme

The MPIE offers outstanding international scientists possibilities to introduce their research topic at any level of their career within the status of a guest. At the same time, guest scientists are given the opportunity to exchange their ideas at an international level with excellent colleagues, thereby establishing important scientific networks.

During 2019-2021 a total of **31** postdoctoral researchers joined the MPIE in frame of the guest programme with a duration of 12-24 months.

Home countries of postdocs in frame of the MPIE guest programme



Scientific honours & appointments

Honours

2018 (not included in the Report 2016 – 2018)

A. Dutta: Winner German Science Slam Championship

F. Roters: Elected to the executive board of the German Materials Society (DGM)

2019

L. Abdellaoui: Graduate Student Conference Registration Wavier for the 38th International Conference on Thermo-electrics

R. Changizi: 1st prize "Arts in Science" image competition, "Microscopy Conference 2019"

A. Dutta: Winner European Science Slam Championship

T. Gänsler: 2nd prize "Electron Microscopy – Physical Sciences" category, image competition of the Royal Microscopical Society

A. Kwiatkowski da Silva: Selected participant in the 69th Nobel Laureate Meeting

N. Peter: Selected participant in the 69th Nobel Laureate Meeting

D. Raabe: Chair of the Gordon Research Conference on Physical Metallurgy at the University of South New Hampshire in Manchester (USA)

D. Raabe: KAIST Lecture Series in Materials Science and Engineering 2019 at the Korea Advanced Institute of Science and Technology KAIST (Korea)

D. Raabe: Bauerman Lecture Award 2019, Imperial College London, Royal School of Mines

I. Souza Filho: Brazilian PhD Award 2019

H. Springer: Friedrich Wilhelm Preis, RWTH Aachen University

M. Stratmann: Re-elected President of the MPG

M. Stratmann: Honorary Member of the Indian Institute of Metals (IIM)

2020

B. Gault: Gottfried Wilhelm Leibniz Award 2020, German Research Foundation (DFG)

MPIE: 1st place in the Alexander von Humboldt Ranking in Engineering Sciences among all non-university research

institutions & 3rd place overall sciences of non-university research institutions

C. Scheu: Elected to the Review Board of the German Research Foundation (DFG)

F. Roters: Re-elected to the executive board of the DGM

H. Zhao: ICAA (International Conference on Aluminium Alloys) Early Career Researcher Award

H. Zhao: TMS Light Metals Subject Award - Aluminum Alloys

S. Zwaka: International Research Marketing Prize, German Research Foundation (DFG)

2021

S. Antonov: Postdoctoral Student Award & the Young Leaders International Scholar - JIM, The Japan Institute of Metals and Materials (JIM) and the Federation of European Materials Societies (FEMS)

R. Aymerich Armengol: Selected participant for the 70th Interdisciplinary Lindau Nobel Laureate Meeting

R. Aymerich Armengol, R. Changizi, A.A. El-Zoka, R. Hosseinabadi and E.I. Saad: Winners of MPIE Science Video Competition Prize

S.H. Kim: Müller Emerging Scientist Award at the Atom Probe Tomography and Microscopy (APT&M) conference

Y. Ma: Walter Benjamin Grant, German Research Foundation (DFG)

Career programmes for female scientists

B. Bellon: Selected to participate in the MPG Sign Up! For Your Career: Earlier postdoc phase in 2022

A. Garzon: Selected to participate in the MPG Sign Up! For Leadership in 2022

O. Kasian: Selected to participate in the MPG Sign Up! Career building for female post docs in 2019

C. Liu: Selected to participate in the MPG Sign Up! For Leadership in 2022

A. Mahajan: Selected to participate in the MPG Sign Up! For Your Career: Earlier postdoc phase in 2022

M. Todorova: Accepted for the Boost! Programme of the MPG in 2020



Fellowships & scholarships

2019

L. Gomell: PhD scholarship of the German Academic Scholarship Foundation

P.-Y. Tung: Taiwanese Government Scholarship to Study Abroad (GSSA)

2020

Z. Wang: FP-RESOMUS Fellowship (Fellowship Program of the NCCR MUST and the Cluster of Excellence RESOLV)

Several of our guest scientists - including all fellows from the Alexander vonHumboldt Foundation - also joined the MPIE with fellowships and schlorships. Please see page 230 onwards for more information.

MPIE trainees

2018 (not included in the Report 2016 – 2018)

T. Freieck: “Chambers best 2018” in the field of materials testing, IHK (chamber of industry and commerce) Düsseldorf (Germany)

2020

A. Laimmer: Max Planck Trainee Award 2020 of the Max Planck Society (Germany)

A. Laimmer: “Chambers best 2020” in the field of materials testing by the IHK (chamber of industry and commerce) Düsseldorf (Germany)

2021

H. Bögershausen, H. Faul, A. Schulz: First place at the Innovationssemester competition of the Wissensregion Düsseldorf e.V.

S. Sprengel: Max Planck Trainee Award 2021 of the Max Planck Society (Germany)

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

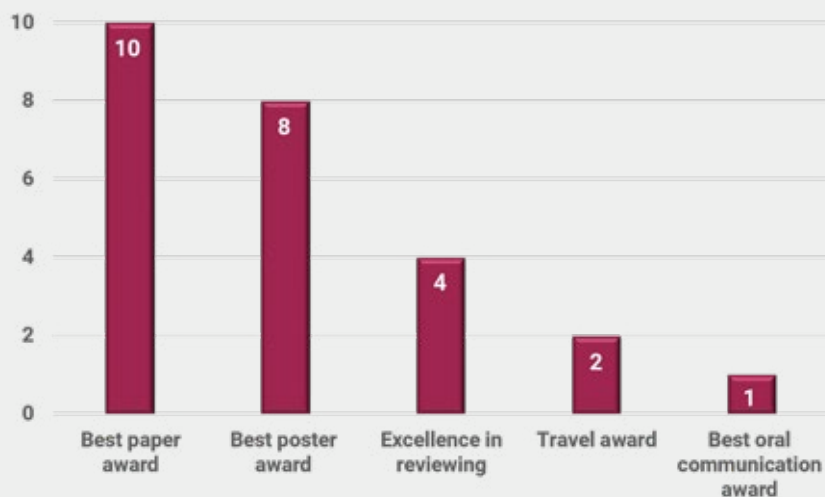
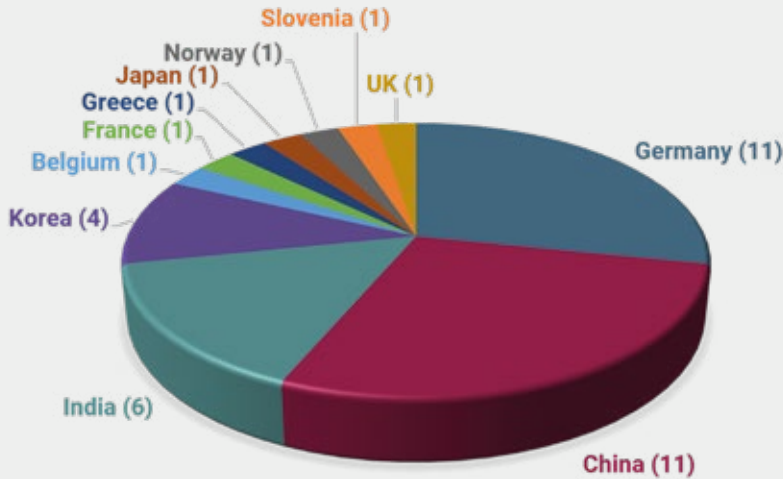


Fig.1: Summary of all best paper, best poster, excellence in reviewing, travel and communication awards received by MPIE scientists between 2019 – 2021. These awards are not listed above.

Appointments

Destination countries of appointments



2018 (not included in Scientific Report 2016 - 2018)

B. Gault: Assistant Professor at the Imperial College London, UK

J. Han: Assistant Professor, Department of Materials Science and Engineering, Chungnam National University, South Korea

O. Kasian: Helmholtz Young Investigator Group at the Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

J. Zavašnik: Member of the Gaseous Electronics Department in the Jožef Stefan Institute (JSI) and Assistant Professor at the Jožef Stefan International Postgraduate School in Ljubljana, Slovenia

2019

H.-O. Fabritius: Full Professor of Bionik und Materialentwicklung, University of Applied Science Hamm-Lippstadt, Germany

X. Fang: Head of the Dislocation Based Functionalities Group within the Ceramics Group in the Department of Materials and Earth Sciences at the Technical University of Darmstadt

P.K. Gokuldoss: Assistant Professor, Indian Institute of Technology Madras, India

J.G. Kim: Assistant Professor, Department of Materials Engineering and Convergence Technology, ReCAPT, Gyeongsang National University, Korea

M. Koyama: Assistant Professor, Tohoku University, Japan

A. Lahiri: Assistant Professor, Metallurgical and Materials Engineering Department, Indian Institute of Technology Roorkee, India

Z. Li: Full Professor, School of Materials Science and Engineering, Central South University, China

W. Lu: Professor, Central South University, China

S.K. Makineni: Assistant Professor, Department of Materials Engineering, Indian Institute of Science, Bangalore, India

Ashish Kumar Saxena: Assistant Professor in the Centre for Innovative Manufacturing Research (CIMR) in the Vellore Campus of the Vellore Institute of Technology (VIT), India

S.S. Sohn: Assistant Professor, Korea University

H. Springer: Professorship at the RWTH Aachen University, Academic and Research Department Metallic Composites, Germany

A. Tripathi: Assistant Professor, Department of Metallurgical and Materials Engineering, Malaviya National Institute of Technology Jaipur, India



Y. Yao: Full professor at the School of Mechanics, Civil Engineering and Architecture at the Northwestern Polytechnical University (NWPUP) in Xi'an, Shaanxi, China

2020

S. Brinckmann: Permanent head of the Micromechanics and Tribology Group at the Forschungszentrum Jülich GmbH, Germany

M. Diehl: Full Professor, Katholieke Universiteit Leuven, Department of Computer Science, Department of Materials Engineering, Belgium

H. Fan: Professor, Associate Chair, Department of Mechanics, Sichuan University, China

M. Ghidelli: Permanent staff scientist position in the Laboratoire des Sciences des Procédés et des Matériaux

(LSPM) at the Université Sorbonne Paris Nord (CNRS), France

W. Guo: Associate Research Fellow in the Research Institute of Aero-Engine at Beihang University in Beijing, China

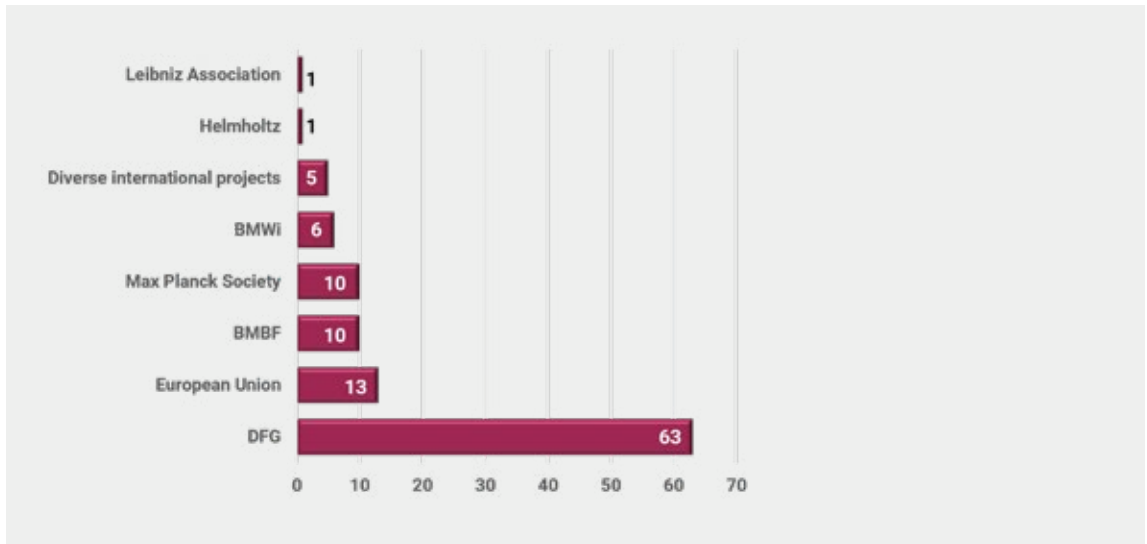
E. Jäggle: Univ.-Prof., Fakultät für Luft- und Raumfahrt-technik Universität der Bundeswehr München, Germany

C. Kirchlechner: Head of the Institute of Biomechanics and Materials at the Karlsruhe Institute of Technology (KIT), Germany

M. Ledendecker: Independent Group Leader at the TU Darmstadt, Germany

D.-H. Lee: Professor, Chungnam National University, Korea

Participation in research programmes 2019 – 2021



National

BMBF

DaNiSh - Development of a high gamma nickel base superalloy with outstanding material properties for applications in drive technology and turbomachinery

MANGAN - Mechanistic investigations of electrochemical oxygen evolution on model electrodes

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

NanoSolar - Semiconducting nanocomposites with tailored optical and electronic properties

Optimization of the efficiency of solar cells based on 3-dimensional chemical analyses on an atomic scale

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

RAVE-K - Resource-saving assembly and connection technology for low-voltage technology contact materials containing precious metals

Stahl*Digital* - Workflows und Plattformintegration

UGSLIT - Ultra high-strength weight-reduced steels for resource-saving lightweight construction in transport applications

White-Etching-Cracks - Knowledge-based design of wear resistant bearing steels by atomic-scale characterization as countermeasure against white-etching crack failure in wind power plants

BMWi

H2BS - New hydrogen barrier coatings for low-cost and high-strength steels in hydrogen technology

MAXCoat - Development of a cost-efficient ferritic bipolar plate with MAX phase corrosion protection for applications in portable and mobile fuel cells

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

PAULL - Activation of ultra-long lifetimes of fuel cells; Subproject: Elucidation of cross-scale degradation mechanisms during electron microscopic characterization of MEAs before and after operation

Pro-FeAl - Process development for economical, efficient turbine components made of iron aluminides (Fe-Al), Subproject C: Alloy design and characterisation

PtTM@HGS - Development of cost-efficient, high performance gas diffusion electrodes for polymer electrolyte membrane fuel cells (PEM-FC) with low Platinum loading and novel hollow graphitic spheres as support

DFG

DFG awards

Gottfried Wilhelm Leibniz Award 2020 for B. Gault

DFG collaborative research centres (SFB), transregio projects (TRR) & priority programmes (SPP)

SFB 761: Steel - Ab Initio. Quantum Mechanics Guided Design of New Fe-based Materials

- A 02: Ab initio thermodynamics und kinetics in the Fe-Mn-Al-C system
- A 07: Microstructure mechanics and fundamentals of concurrent twinning and martensite formation
- A 09: Ab initio based mesoscale simulation of hydrogen embrittlement
- C 01: Microstructure analytics
- C 04: Fatigue, damage and stress corrosion cracking under cyclic loading
- C 05: Defects and Stresses in Fe-Mn-C Steels
- C 08: 3D atomic analysis of the local chemical composition by atom probe tomography
- C 10: Deformation behavior of multi-phase steels
- T 07: Liquid metal embrittlement by Zn in Mn-containing steels with significant austenite content

SFB 1232: From colored states to evolutionary structural materials

- S02: Correlative study towards experimental validation of the high throughput methodology

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

- A01: Solid solution effects on dislocation activity
- A02: Atomistic simulations of dislocation processes
- A06: Ab initio accuracy on large scales using machine learning
- B01: Interfaces in Mg-Al-Ca alloys in dependence on chemical composition and temperature
- B04: Corrosion of Mg alloys and intermetallics
- B06: Fracture of complex intermetallic phases: influence of temperature
- C01: Multiphysics description of Mg composites at the grain scale
- C05: Ab initio thermodynamics of defect phases

SFB/ TRR 188: Damage Controlled Forming Processes

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

TRR 103: From Atoms to Turbine Blades – A Scientific Approach for Developing the Next Generation of Single Crystal Superalloys

- A04: Investigation of the local alloy composition by atom probe tomography

TRR 270: HoMMage - Hysteresis design of magnetic materials for efficient energy conversion: HoMMage

Priority programmes

SPP 1239: Modification of Microstructure and Shape of Solid Materials by External Magnetic Fields: Ab initio investigation of temperature dependent effects in magnetic shape memory Heusler alloys

SPP 1568: Design and Generic Principles of Self-healing Materials

- Towards self-healing metals by employing optimally-dispersed Ti-Ni Shape-memory nano-particles

SPP 1594: Topological Engineering of Ultra-Strong Glasses

- Quantum mechanically guided design of ultra-strong and damage-tolerant glasses

SPP 1613: Regeneratively Produced Fuels by Light Driven Water Splitting: Investigation of Involved Elementary Processes and Perspectives of Technologic Implementation

- Metal oxide nanostructures for electrochemical and photoelectrochemical water splitting

SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials

- Evolution of strengthening phases under in-service stresses and temperatures: phase-field and experimental study
- Mechano-chemical coupling during precipitate formation in Al-based alloys
- Phase-field-based chemomechanical models for phase transitions and dislocation-microstructure interaction in metallic alloys with application to kappa-carbides
- Thermo-chemo-mechanical coupling during thermo-mechanical processing of microalloyed steels

SPP 1839: Tailored Disorder - A science- and engineering-based approach to materials design for advanced photonic applications: Broadband reflecting fibers with tailored structures inspired by desert ants

SPP 1959: Manipulation of matter controlled by electric and magnetic fields: Towards novel synthesis and processing routes of inorganic materials

- Electro-plasticity in Al-Cu eutectic alloys
- Micromechanisms of the electro-plastic effect in magnesium alloys investigated by means of electron microscopy

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

- MarioCCArt - Mechanical properties and hydrogen tolerance of particle-reinforced CCA produced by additive manufacturing
- MULTI TRIP CCA-s – Design and mechanical properties of compositionally complex alloys from twinning-induced towards bidirectional transformation-induced plasticity
- PaCCman - Particle-strengthened Compositionally Complex Alloys - interlinking powder synthesis, additive manufacturing, microstructure evolution and deformation mechanisms
- Tailored precipitation (B₂, L₂,) strengthened, compositionally complex FeAlCr (Mn, Co, Ni, Ti) alloys for high temperature applications

FOR 1700: Metallic Nanowires on the Atomic Scale: Electronic and Vibrational Coupling in Real World Systems

DFG research grants

Ab initio based calculation of the stability of selected TCP precipitates in steels: Temperature and interface effects

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

Additive Manufacturing - Precipitation kinetics during non-linear heat treatment in Laser Additive Manufacturing

AHEAD - Analysis of the Stability of High Entropy Alloys by Dewetting of Thin Films

Automated analysis and validation of interatomic potentials for application in Materials Science

Can high strength and moderate ductility be combined in wear resistant coatings? A fundamental plasticity study of X₂BC nanolaminates (X=Hf, MO)

Characterization and modeling of the interplay between grain boundaries and heterogeneous plasticity in titanium

Consistent physically-based modeling of dynamic recrystallization under hot working conditions

CORRKEST - Correlative Characterization of co-evaporated Cu₂ZnSnSe₄- thin films

Correlation of growth, structure, optical and electronic properties of novel Nb₃O₇(OH) and Nb₂O₅ nanostructures

C-Tram - Atomic scale redistribution of carbon during the transformation from austenite to martensite in steels

Diffusion in high entropy alloys: Development and application of an experiment-ab initio approach

Elementary mechanisms of tribologically-induced oxidation in copper

Exploring Multinary Nanoparticles by Combinatorial Sputtering into Ionic Liquids and Advanced Transmission

Electron Microscopy

Fracture initiation in FCC and BCC metals during tribology

From interatomic potentials to phase diagrams: Integrated tools for validation and fitting

Hydrogen-microstructure interactions in iron-based alloys at small scales: from amorphous, via nanocrystals, to polycrystals

MAGIKID - Magnetism in iron alloys: thermodynamics, kinetics and defects

Metallic glasses - Structure, phase formation and properties of metallic glasses manipulated by electric current

Mxene – Mxene-based energy materials guided by 3D Atomic-Resolution Tomography

RE-MAP - Rare-earth based alloys for hard-magnetic applications: Temperature and pressure dependent phase stabilities

Spektralmethoden / KugelRVE - Spectral methods for spherical representative volume elements

Structure, phase formation and properties of metallic glasses manipulated by electric current

Study of grain-boundary-dislocation interactions by advanced in situ μ Laue diffraction

XMicrFatigue - X-ray Laue Microscopy to Understand Fatigue Damage

DFG cluster of excellence

Stability of electrode materials in an electrochemical environment”, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation)

DFG competition on international research marketing

Coffee with Max Planck: Research Opportunities at the MPIE



Max Planck Society

Combinatorial design of novel rare-earth free, high-entropy based permanent magnets

Designing Damage Tolerant Functional Oxide Nanostructures: Damage Tolerance Studies on Barium Titanate at Small Length Scales

Environmental Degradation of High-Temperature Materials in Service Conditions

International Max Planck Research School for Interface Controlled Materials for Energy Conversion IMPRS SurMat (IMPRS - SurMat)

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

BiGmax project: Investigation of deep learning-based approaches to solve partial differential equations in mechanical equilibrium problems

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

Max Planck Fellow Group Self-Reporting Materials (Jochen Schneider)

Microstructure Design of High-Performance Materials for Harsh Energy Applications

Stress and defects driven phase transformations

Helmholtz

Helmholtz school for data science in life, earth, and energy (HDS-LEE)

Machine Learning Enhanced Multi-Scale Modeling of Ice Deformation and Melting

Leibniz Association

CarMON - New Carbon-Metal Oxide Nanohybrids for Efficient Energy Storage and Water Desalination

International

European Union

ERC (European Research Council)

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

SHINE - Seeing hydrogen in matter

TIME-BRIDGE - Time-scale bridging potentials for realistic molecular dynamics simulations-TIME-BRIDGE

Marie Skłodowska-Curie Actions

smartCC - Designing novel smart sensor interfaces based on a biologically abundant peptide motif

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

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

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

UltimateGaN - Technologies for novel power electronics and radar applications; Subproject: Identification of degradation and failure mechanisms and optimisation of novel nitride-based power electronics devices by ab initio simulations

RFCS (Research Fund for Coal and Steel)

DELIGHTED - Design of Lightweight Steels for Industrial Applications

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

MicroCorr - Improving steel product durability through alloy coating microstructure

MuSTMeF - Multi Scale Simulation Techniques for Metal Forming



FFG (Austrian Research Promotion Agency)

Fundamentals and tools for integrated computational modeling and experimental characterization of materials in the atomic to micrometer scale range", Project A1.23 (COMET II) / Project P1.1 (COMET III)

FWO - Fonds Wetenschappelijk Onderzoek

PredictCor - Knowledge and technology platform for prediction of durability and lifetime of organic coated metals under long-term environmental corrosion

M2i

DENS - Digitally Enhanced New Steel Product Development

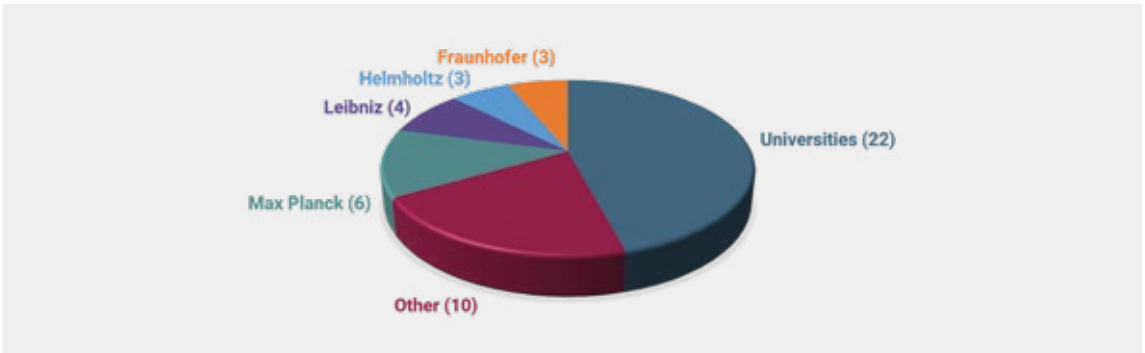
- T17019o "Full field simulation of Dynamic Recrystallization"
- T17019e "Multi-field RVE simulation"

NWO (Dutch Research Council)

Systematic simulation of high-entropy alloys

Collaboration with national and international universities and research institutes

National



Universities

- | | |
|---|---|
| Brandenburgische Technische Universität Cottbus-Senftenberg | Technische Universität Darmstadt |
| Bergische Universität Wuppertal | Technische Universität München |
| Friedrich-Alexander-Universität Erlangen-Nürnberg | Universität Bayreuth |
| Heinrich-Heine-Universität Düsseldorf | Universität Bielefeld |
| Karlsruher Institut für Technologie - KIT | Universität Bremen |
| Ludwig-Maximilians-Universität | Universität Duisburg-Essen |
| Otto-von-Guericke-Universität Magdeburg | Universität Konstanz |
| Ruhr-Universität Bochum | Universität Paderborn |
| RWTH Aachen | Universität Siegen |
| Technische Universität Bergakademie Freiberg | Universität Stuttgart |
| Technische Universität Clausthal | Westfälische Wilhelms-Universität Münster |

Research institutes

- | | |
|---|---|
| Access e. V. | Institut für Angewandte Informatik e.V. (InfAI), Leipzig |
| Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin | Institut für Energie- und Umwelttechnik e.V. (IUTA), Duisburg |
| Deutsche Akademie der Naturforscher Leopoldina, Halle | Fraunhofer Institut für Lasertechnik (ILT), Aachen |
| Deutsches Zentrum für Luft- und Raumfahrt (DLR), Bonn | Fraunhofer Institut für Werkstoffmechanik (IWM), Freiburg |
| fem Forschungsinstitut Edelmetalle + Metallchemie, Schwäbisch Gmünd | Fraunhofer-Institut für Werkstoff- und Strahltechnik (IWS), Dresden |
| Forschungszentrum Jülich GmbH | |

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: Institut für Werkstoffphysik, Geesthacht

Leibniz-Institut für Festkörper- und Werkstofforschung (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 Physik fester Stoffe, Dresden

Max-Planck-Institut für Festkörperforschung, Stuttgart

Max-Planck-Institut für Intelligente Systeme, Stuttgart

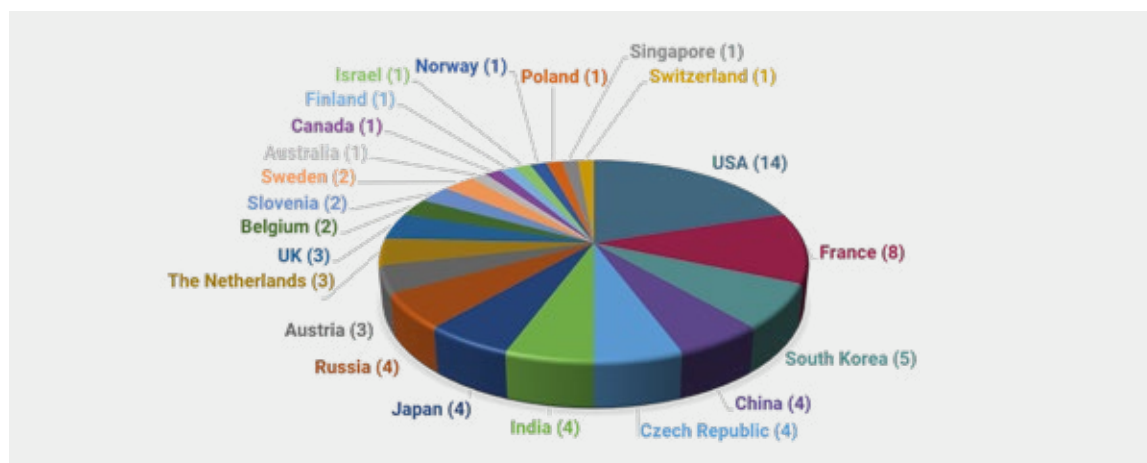
Max-Planck-Institut für Kohlenforschung

Max-Planck-Institut für Chemische Energiekonversion

VDEh-Betriebsforschungsinstitut GmbH (BFI), Düsseldorf

Zentrum für Brennstoffzellen-Technik GmbH, Duisburg

International



Universities

Aix-Marseille University, France

Beijing Institute of Technology, China

Belgorod State University, Russia

Brown University, Providence, Rhode Island, USA

Central South University, Changsha, China

Charles University Prague, Czech Republic

Clemson University, South Carolina, USA

Delft University of Technology, The Netherlands

Ecole Polytechnique, France

Hasselt University, Belgium

Hokkaido University of Science, Sapporo, Japan

Imperial College London, UK

Indian Institute of Technology Bombay, India

Indian Institute of Technology Chennai, India

Indian Institute of Technology Madras, India

Kangwon National University, Chuncheon, South Korea

Katholieke Universiteit Leuven, Belgium

Korea University, Seoul, South Korea

KTH Royal Institute of Technology, Stockholm, Sweden

Leiden University, The Netherlands

Linköping University, Sweden

MINES ParisTech, PSL - Research University, France

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

Silesian University of Technology, Gliwice, Poland

Singapore University of Technology and Design, Singapore

Southern University of Science and Technology, Shenzhen, China

Tampere University, Finland

Technical University Eindhoven, The Netherlands

Technical University Liberec, Czech Republic

Tongji University, Shanghai, China

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 Florida, Gainesville, USA

University of Illinois, USA

University of Manchester, UK

University of Oxford, UK

University of Ulsan, South Korea

University of Vienna, Austria

University of West Bohemia, Pilsen, Czech Republic

UNSW Sydney, Australia

Research institutes

Academy of Sciences of the Czech Republic, Brno, Czech Republic

Austrian Academy of Sciences, Leoben, Austria

CEA Saclay, Paris, France

Centre de Mise en Forme des Matériaux (CEMEF), Nice, France

Centre National de la Recherche Scientifique (CNRS): Office National d'Etudes et de Recherches Aérospatiales (ONERA), Châtillon, France

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

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

Institut de Physique et Chimie de Matériaux de Strasbourg, France

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

Institute of Quantum Materials Science, Yekaterinburg, Russia

Jožef Stefan Institute, Ljubljana, Slovenia

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

Korea Institute for Industrial Technology, 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

Massachusetts Institute of Technology (MIT), Cambridge, Massachusetts, USA

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

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

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

Collaborating industrial partners and patents

National

BMW Group AG	MTU Aero Engines AG
Deloro Wear Solutions GmbH	Otto Junker GmbH
DHS – Dillinger Hütte Saarstahl AG	point electronic GmbH
Dr. Kochanek Entwicklungsgesellschaft	Robert Bosch GmbH
Freudenberg Sealing Technologies, Freudenberg FST GmbH	Rolls-Royce Deutschland Ltd & Co KG
Heraeus Deutschland GmbH & Co. KG	Salzgitter Mannesmann Forschung GmbH
Infineon Technologies AG	Schott AG
Innovationsgesellschaft für fortgeschrittene Produktionssysteme GmbH (inpro)	Siemens AG
KSB Stiftung	Speira GmbH, Research & Development
Leistritz Turbinentechnik GmbH	thyssenkrupp Steel Europe AG
Materials Science International Services GmbH (MSI)	VDM Metals International GmbH, Research and Development
	Volkswagen AG

International

AMAG Austria Metall GmbH, Austria	Kobe Steel, Ltd., Japan
Alemnis, Switzerland	Materials Center Leoben Forschungs GmbH, Austria
Denso Corporation KK, Japan	Rolls-Royce Motor Cars Ltd, England
ELHCO - Electroless Hard Coat S.A., Spain	Sandvik Coromant R&D, Sweden
Exaddon AG, Switzerland	Tata Steel Nederland Technology BV, The Netherlands
Infineon Technologies Austria AG, Austria	Thermo-Calc Software AB, Sweden
JFE Steel Corporation, Japan	Vallourec Research Center France, France
KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH, Austria	Wärtsilä Finland Oy, Finland
	Winterthur Gas & Diesel Ltd, Switzerland



Patents

Patents issued in the given time schedule

Date of Issue	Description	Inventors
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 06, 2021	Process for recycling of noble metals USA 15/771,500 EP 3368698	Mayrhofer, Karl Hodnik, Nejc Baldizzone, Claudio

Patents filed in the given time schedule

Date of Pending	Description	Inventors
October 9, 2018	Temperature Measurement for a High Temperature Micro-deformation Device (EP 18199374.2.)	Arigela, Viswanath Gowtham Kirchlechner, Christoph Gonzalez, Iwan Kölling, Michael

Patents - overview

Date of issue	Description	Inventors
June 05, 2015	Korrosionsbeständiger TWIP-Stahl (JP 2011-553279.)	Weber, Sebastian Mujica Roncery, Lais
June 07, 2018	Fabrication of nanoporous carbide membranes Joint invention with Universitat Politecnica de Catalunya (EP 2 664 683)	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 Taipe, who is applicant (TWI490487)	Erbe, Andreas Chia-Fu Chu Ming-Li Chu Leonardo Lesser-Rojas, all Academia Sinica, Taipe
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
October 25, 2016 October 27, 2015	Process for recycling of noble metals (DE 102015118279.3) (PCT/ DE2016/ 100498; EP 3 368 698)	Mayrhofer, Karl Hodnik, Nejc Baldizzone, Claudio
January 31, 2013 May 19, 2009	Hochfester C-Stahl mit Superplastizität Joint invention with Daimler Chrysler (DE 10 2005 027 258.4) (US 7.534314B2)	Frommeyer, Georg Gerick, Arndt Haug, Tilmann, Kleinkathöfer, Wolfgang, all DaimlerChrysler AG

Conferences, symposia and meetings organized by the institute

2018 (not included in the Scientific Report 2016 - 2018)

L. Stephenson co-organized and chaired a session at the "International Microscopy Conference (IMC)", Sydney (Australia), 09 – 14 Sep 2018

L. Stephenson co-organized the "European Atom Probe Workshop (EAPW)" at the MPIE, Düsseldorf (Germany), 07 – 09 Nov 2018

2019

F. Stein organized the "International Workshop on Laves Phases" at the MPIE, Düsseldorf (Germany), 14 - 15 Jan 2019

S. Brinckmann, G. Dehm, and C. Scheu organized the Symposium "Mechanics Meets Energy 2019" in Cuxhafen (Germany), 21 - 25 Jan 2019

F. Stein and M. Palm co-organized the "3rd MSIT Winter School on Materials Chemistry" at Ringberg Castle, Kreuth (Germany), 03 - 06 Mar 2019

F. Körmann co-organized the Topical Session "High entropy and compositionally complex alloys" at the DPG Spring Meeting 2019 in Regensburg (Germany), 01 - 05 Apr 2019

C. Liebscher, F. Körmann, B. Grabowski, and S. Divinski organized the symposium "High entropy and compositionally complex alloys" at the DPG Spring Meeting 2019 in Regensburg (Germany), 01 - 05 Apr 2019

J. Neugebauer co-organized the Topical Session "Symposium "Big data analysis in Materials Science" at the DPG Spring Meeting 2019 in Regensburg (Germany), 01 Mar - 05 Apr 2019

B. Gault was the IFES (International Field Emission Society) Chair for "Microscopy & Microanalysis 2019" in Portland, OR (USA), 04 - 08 Aug 2019

G. Dehm co-organized the symposium "Metals, Alloys and Intermetallics" at the Microscopy Conference MC2019, Berlin (Germany), 01 - 05 Sep 2019

F. Körmann co-organized the workshop "Conference on Theory of Complex Disorder in Materials" at the Linköping University, Linköping, (Sweden), 16 - 18 Sep 2019

M. Palm and F. Stein co-organized the international conference "Intermetallics 2019" at the Educational Center Kloster Banz, Bad Staffelstein (Germany), 30 Sep - 04 Oct 2019

G. Dehm, C. Liebscher, C. Scheu, and B. Völker organized the „International Workshop on Advanced In Situ Microscopies of Functional Nanomaterials and Devices – IAMNano 2019" at MPIE, Düsseldorf (Germany), 27 - 30 Oct 2019

B. Gault, T. Schwarz, and L. Gomell co-organized the "NRW Atom probe user meeting" at the MPIE, Düsseldorf (Germany), 07 Nov 2019

M. Rohwerder organized the 9th GfKORR Work Group Meeting „Korrosionsuntersuchung und Überwachung" and the 8th GfKORR Work Group Meeting "Grundlagen und Simulation" at the MPIE, Düsseldorf (Germany), 21 Nov 2019

2020

S. Brinckmann, G. Dehm, and C. Scheu organized the Symposium "Mechanics Meets Energy 2020" in Lingen (Germany), 13 - 17 Jan 2020

G. Dehm, C. Kirchlechner, and U. Hangen organized the "Nanobrücken 2020: A Nanomechanical Testing Conference", Düsseldorf (Germany), 04 - 06 Feb 2020

F. Stein and M. Palm co-organized the "4th MSIT Winter School on Materials Chemistry" at Ringberg Castle, Kreuth (Germany), 16 - 20 Feb 2020

J. Janssen, S. Surendralal, J. Neugebauer, Y. Lysogorskiy, and R. Drautz, organized the piron Virtual Workshop "Workflows for atomistic simulations", Düsseldorf (Germany), 15 - 17 Apr 2020

M. Ashton, M. Todorova, J. Neugebauer, organized the Workshop „Electrically triggered reactions at interfaces – from *ab initio* to the multiscale", Schloss Ringberg (Germany), 26 – 29. Apr 2020. Cancelled due to COVID-19.

A. A. El-Zoka, co-chaired the sessions "L04-Metal Organic Frameworks" and "L04-Nanoporous Materials by Dealloying" at the 237th ECS Meeting within the 18th International Meeting on Chemical Sensors, Sensors, held online, 30 May - 03 Jun 2020

D. Raabe, J. Neugebauer, M. Kühbach, C. Freysoldt, B. Gault, and C. Liebscher organized the online „BiGmax Workshop 2020 on Big-Data-Driven Materials Science", held online, 15 - 16 Jun 2020

B. Gault, T. Schwarz, and L. Gomell co-organized the "NRW Atom probe user meeting" at the MPIE Düsseldorf (Germany), 23 June 2020

L. Abdellaoui organized the "1st Virtual Thermoelectric Conference 2020" (VCT 2020), 21 - 23 July 2020



C. Scheu co-organized the “International Seminar Series on the Microstructure of Materials”, held online, 10 Sep 2022

M.J. Duarte, M. Herbig, J. Sietsma, and R. Petrov organized the symposium “Material Response to Complex Mechanical and Chemical Loading” at the MSE 2020 conference, held online, 22 - 25 Sep 2020

M. Herbig organized the symposium “Material Response to Complex Mechanical and Chemical Loading” at the MSE 2020 conference, held online, 22 - 25 Sep 2020

L. Huber co-organized the symposium “Predicting Interface Structure and Dynamics” at the Materials Science and Engineering (MSE) Congress, held online, Darmstadt (Germany), 22 - 25 Sep 2020

C. Liebscher, C. Kübel, and P. van Aken organized the symposium “Advanced Transmission Electron Microscopy for Materials Science” at the MSE 2020 conference, held online, 22 - 25 September 2020

F. Stein and M. Palm organized the International Conference “TOFA 2020 - 17th Discussion Meeting on Thermodynamics of Alloys” at the Educational Center Kloster Banz, Bad Staffelstein (Germany), 28 Sept - 03 Oct 2020

T. Hickel, J. Neugebauer, R. Drautz, and F. Soisson organized the “Ab initio Description of Iron and Steel (ADIS2020)” Workshop “Diffusion and Precipitation”, Schloss Ringberg (Germany), held online, 02 - 05 Nov 2020

R. Otis, J. Janssen, T. Hickel, J. Neugebauer, B. Bocklund, and Z.K. Liu organized the Workshop “Software Tools from Atomistics to Phase Diagrams”, held online, 10 - 11 Nov 2020

2021

M. Todorova and N. Hörmann, organized the mini-Symposium “Electrified Solid - Liquid interfaces” at the Online

Spring Meeting of the Surface Science Division of the German Physical Society (DPG), 01 - 04 Mar 2021

Y. Lysogorskiy, R. Drautz, S. Surendralal, J. Janßen, and J. Neugebauer, organized the Workshop “Workflows for Atomistic Simulations”, held online, 10 - 12 Mar 2021

S. Antonov co-organized the “Defect and Phase Transformation Pathway Engineering for Desired Microstructures” at TMS 2021 Annual Meeting, held online, 15 - 18 Mar 2021

G. Dehm, C. Gammer, Sang Ho Oh, and K.Y. Xie organized the symposium “In-situ mechanical testing of materials at small length scales, modelling and data analysis” at the 2021 MRS Virtual Spring Meeting, held online, 17 - 23 Apr 2021

B. Gault and L. Gomell co-organized the “NRW Atom probe user meeting” at the MPIE, Düsseldorf (Germany) 28 - 29 Apr 2021

M.J. Duarte, M. Cordill, and M.T. Lin organized the symposium “Mechanical Properties and Adhesion” at the 47th International Conference on Metallurgical Coatings & Thin Films (ICMCTF 2020), held online, 26 - 30 Apr 2021

F. Stein and M. Palm co-organized the “5th MSIT Winter School on Materials Chemistry”, held online, 02 - 06 May 2021

C. Freysoldt, C. Liebscher, and R. Ernstorfer organized the online BiGmax summer school “Harnessing big data in materials science from theory to experiment”, 13 - 17 Sep 2021

M. Palm and F. Stein co-organized the international conference “Intermetallics 2021” at the Educational Center Kloster Banz, Bad Staffelstein (Germany), 04 - 08 Oct 2021

M. Rohwerder co-organized the “C03 - Corrosion Mechanisms and Methods” symposium at the 240th Meeting of the ECS, held online, 10 - 14 Oct 2021

Institute colloquia and invited seminar talks

2019

Liang Gao, Max Planck Institute for Plasma Physics, Munich, Germany: Interaction of Deuterium Plasma with Tungsten: With Focus on Hydrogen-Induced Damage (03 Jan 2019)

Stefan Pogatscher, Montanuniversität Leoben, Leoben, Austria: Phase Transitions in Non-Equilibrium Metallic Systems (18 Jan 2019)

Andrea Brognara, Politecnico di Milano, Milan, Italy: Synthesis and Integration of Nanostructured TiO₂ Films with Plasmonic Au Nanoparticles (18 Jan 2019)

Felix Gunkel, Institute of Electronic Materials, RWTH Aachen University, Aachen, Germany and Peter Gruenberg Institut (PGI-7) – Forschungszentrum Jülich, Jülich, Germany: Nanoscale Thermodynamics at Complex Oxide Surfaces and Interfaces for Application in Electronics, Sensing, and Energy Conversion (31 Jan 2019)

Minoru Otani, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan: Theoretical Description of the Equilibrium Potential of an Electrochemical Reaction on a Metal Electrode (05 Feb 2019)

Timon Rabczuk, Bauhaus University Weimar, Weimar, Germany: Computational Modeling of Moving Boundary Problems (07 Feb 2019)

Bianca Maria Colosimo, Politecnico di Milano, Milan, Italy: In-situ Sensing and Monitoring of Metal Additive Manufacturing Processes (11 Feb 2019)

Jean-Sébastien Micha, European Synchrotron Radiation Facilities (CEA-INAC: CRG-IF at BM32), Grenoble, France: Facilities and Capabilities of French CRG-IF BM32 Beamline to Study Materials (11 Feb 2019)

Stéphane Berbenni, Vincent Taupin, Université de Lorraine, Metz, France: A Micromechanical Approach Based on Fourier Transforms and Continuum Dislocation Mechanics to Simulate Grain Size Effects in Polycrystals (18 Mar 2019)

Antoine Guitton, Université de Lorraine, Metz, France: Accurate Electron Channeling Contrast Imaging (aECCI): A Powerful Tool for Understanding the Fundamental Deformation Mechanisms of Materials (18 Mar 2019)

Sang Ho Oh, Sungkyunkwan University, Seoul, Republic of Korea: TEM Studies on Materials with a Negative Poisson's Ratio (21 Mar 2019)

Claudia Felser, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany: The Heusler System (for Thermoelectric Application): How You Can Use the Periodic Table as a Lego Box to Build the States You Are Interested in (9 Apr 2019, Colloquium)

Henry Ovri, Helmholtz Zentrum Geesthacht, Geesthacht, Germany: Nanoindentation Based Investigations of PLC-type Plastic Instability (11 Apr 2019)

Gabi Schierning, Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Dresden Germany: Making Quantum Transport Visible in Thermoelectric Bi₂Te₃ Nanoparticles (24 Apr 2019)

Ondrej L. Krivanek, Nion R&D, Kirkland, WA, and Arizona State University, Tempe, AZ, USA: Aberration-corrected STEM and Ultra-high Energy Resolution EELS (6 May 2019)

Thomas D. Swinburne, CNRS, CINA, Marseille, France: Multiscale Materials Modelling using Sampling and Statistical Mechanics (7 May 2019)

Christian Greiner, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany: Deformation Mechanisms in Metals under a Tribological Load (16 May 2019)

Jakob Schwiedrzik, Empa - Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland: Micromechanics of Bone: Fundamental Research and Clinical Applications (17 May 2019)

Viet Anh Ha, Université catholique de Louvain (UCL), Louvain-la-Neuve, Belgium: High throughput computing for high mobility p-type transparent conducting materials (22 May 2019)

Natasha Stephens, Plymouth Electron Microscopy Centre, University of Plymouth, UK: Exploring the Solar System; From the Nano to Astronomical Scale (4 June 2019, Colloquium)

Aleksandar Zeradjanin, Universität Bremen, Germany: What is the trigger for hydrogen evolution reaction? (5 June 2019)

Ümit Güder, Çanakkale Onsekiz Mart University, Turkey: History of Iron Metallurgy in Anatolia (24 June 2019)

Ivan Kaban, Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Dresden Germany: Experimental studies of phase formation and microstructure development upon non-equilibrium solidification (28 June 2019)

Moritz to Baben, GTT-Technologies, Aachen, Germany: The High-Throughput Way from 0 K to Relevant Temperatures to Enable the Circular Economy (2 July 2019)

Paul Coxon, University of Cambridge, Cambridge, UK: A Sustainable Molten Salt Route for the Electro-extraction and Electro-refining of Low-grade Ores to Yield High Purity Titanium Powders (4 July 2019, Colloquium)

Dominik Noeger, Montanuniversität Leoben, Leoben, Austria: Interaction of the H₂ molecule with carbon nanostructures: A DFT study (17 July 2019)



Yolita Eggeler, University of California, Santa Barbara, CA, USA: Using Analytical Electron Microscopy to Study Microstructural Evolution and Its Effect on Structural & Functional Properties (19 July 2019)

Björn Grüning, University of Freiburg, Germany: Integrative Data Analysis - Building Frameworks to Serve the 21st Century Data Science Problems (31 July 2019)

Hung-wei (Homer) Yen, National Taiwan University, Taipei, Taiwan: Machine Learning Enabled Materials Design: Low-Modulus Ti Alloys (22 Aug 2019)

Tobias Brink, EPFL - École Polytechnique Fédérale de Lausanne, Switzerland: Molecular Dynamics Simulations and Beyond for Plasticity and Wear of Metals (27 Aug 2019)

Erik Bitzek, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany: Towards a More Realistic Modeling of Defect-Defect Interactions in Atomistic Simulations of Crystalline Materials (5 Sept 2019)

Binglun Yin, École polytechnique fédérale de Lausanne, Lausanne, Switzerland: Yield Strength and Misfit Volumes of NiCoCr and Implications for Short-Range-Order (18 Sept 2019)

Taher Saif, University of Illinois at Urbana-Champaign, IL, USA: Lessons Learned from Nano Scale Specimens Tested by MEMS Based Apparatus (24 Sept 2019)

John Wheeler, University of Liverpool, UK: Interactions of Stress with Chemical Processes in Crystalline Materials (26 Sept 2019, Colloquium)

Zi-Kui Liu, Pennsylvania State University, State College, PA, USA: Where Do Thermodynamics and Transport Kinetics Meet? (27 Sept 2019)

Uwe Glatzel, University of Bayreuth, Bayreuth, Germany: Close Packed Phases in Nickel-Based Superalloys - Investigation by Diffusion Multiples (30 Sept 2019)

Mehmet Acet, University of Duisburg-Essen, Duisburg, Germany: Inducing Strong Magnetism in High-Entropy Alloys by Exploiting Their Anti-Invar Properties (8 Oct 2019)

Dietmar Hömberg, WIAS & Institut für Mathematik, TU Berlin, Germany: Mathematics for Steel Production and Manufacturing (14 Oct 2019)

Benjamin Balke, Fraunhofer Research Institution for Materials Recycling and Resource Strategies IWKS, Hanau, Germany: Designing Thermoelectric Highly Efficient H-Free n- & p-type Heusler Compounds via Phase Separation and Nano-Composites (17 Oct 2019)

James P. Best, RWTH University Aachen: Multi-Scale Design and Analyses of Advanced Materials: Experimental Approaches (17 Oct 2019)

Peter Schweizer, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany: Manipulation of Individual Defects in 2D and Layered Materials (18 Oct 2019)

Rajaprakash Ramachandramoorthy, EMPA, Thun, Switzerland: Pushing the Boundaries of Micro and Nanomechanics (22 Oct 2019)

Nesma Aboulkhair, Centre for Additive Manufacturing (CfAM), University of Nottingham, Nottingham, UK: An Approach to Powder Feedstock Modification for *in-situ* Alloying in Metal Additive Manufacture to Improve the Processability of Difficult-to-Process Materials using Carbon Nanotubes (31 Oct 2019)

Marco Simonelli, Centre for Additive Manufacturing (CfAM), University of Nottingham, Nottingham, UK: Development of Novel Titanium Alloys for Laser Powder Bed Fusion (31 Oct 2019)

Masaaki Sugiyama, Osaka University, Japan: Use of Focused Ion Beam (FIB) Instruments for TEM Sample Preparation and Standardization of FIB Processes (07 Nov 2019)

Michael Farle, University of Duisburg-Essen, Duisburg: Novel Magnetic Functionalities in Classic Materials (11 Nov 2019, Colloquium)

Jürgen Bär, Bundeswehr University Munich: Investigation of Thermal Effects in Cyclic Loaded Metallic Materials (20 Nov 2019)

Marvin Poul, University of Stuttgart, Stuttgart, Germany: From Atom Probe Tomography to CALPHAD modeling: Estimating T_c from local concentration fluctuations (26 Nov 2019)

Szylvia Kalácska, Empa Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland: Characterization of Plastically Deformed Metals by 3D High Resolution Electron Backscatter Diffraction (HR-EBSD) at the Micron Scale (11 Dec 2019)

2020

Michael W. Finnis, Imperial College London, London, UK: Interactions of H with vacancies in Fe (15 Jan 2020)

Stefan Sandfeld, TU Bergakademie Freiberg, Freiberg, Germany: Software solutions for micromechanical materials modeling (16 Jan 2020)

Nima H. Siboni, Technische Universität Berlin, Berlin, Germany: Non-Monotonic Rheology of a Magnetic Liquid Crystal System in an External Field (16 Jan 2020)

Christian Silbermann, Technische Universität Chemnitz, Chemnitz, Germany: On the modeling of dislocation- and deformation-induced plastic localization phenomena of metallic materials (28 Jan 2020)

Motomichi Koyama, Tohoku University, Sendai, Japan: Effects of Dislocation Planarity and Compositional Complexity on Hydrogen Embrittlement of Austenitic Steels (17 Feb 2020)

Louis Vanduyffhuys, University of Ghent, Ghent, Belgium: Unraveling the thermodynamic conditions for negative gas adsorption in soft porous crystals (17 Feb 2020)

Erik Bitzek, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen: Influence of Deformation-Induced Topological Anisotropy on Mechanical Properties of Silica Glass: An Atomistic Study (18 Feb 2020)

Jeffrey Snyder, Northwestern University, Evanston, IL, USA: Engineering Defects and Grain Boundaries in Thermoelectric Materials (21 Feb 2020, Colloquium)

Yang Bai, Technical University Darmstadt, Darmstadt, Germany: Chemo-Mechanical Modeling of the Diffusion and Fracture in Cathode Materials of Lithium-Ion Batteries (27 Feb 2020)

Güven Kurtuldu, ETH Zurich, Zurich, Switzerland: Quasicrystal-Induced Nucleation Mechanism in Undercooled Liquids (14 July 2020)

Hortense Le Ferrand, Nanyang Technological University, Singapore: Bioinspired Multifunctional Structural Materials (13 Aug 2020)

Ralf Drautz, ICAMS, Bochum, Germany: Atomic cluster expansion for accurate and transferable interatomic potentials (24 Aug 2020)

Megan Cordill, Eric Schmid Institute of Materials Science, Leoben, Austria: Evaluating Electro-Mechanical Reliability using *in-situ* Methods (27 Aug 2020)

Gaurav Mohanty, Tampere University, Tampere, Finland: Reliable Extraction of Deformation Activation Parameters from Transient and High Strain Rate Micromechanical Tests (10 Sept 2020)

Stefan Pauliuk, University of Freiburg, Freiburg, Germany: Sustainability Challenges in the Global Steel Cycle (21 Oct 2020)

Jean-Philippe Couzinié, Université Paris Est, Paris, France: Insights into the Exploration of Refractory High-Entropy Alloys: From the Design to the Deformation Mechanisms of these Complex Materials (6 Nov 2020)

Vanessa Wood, ETH Zurich, Zurich, Switzerland: Volumetric Imaging for Better Batteries (19 Nov 2020, Colloquium)

Samuel Forest, Mines ParisTech, Paris, France: A Cosserat crystal plasticity and phase field approach to grain boundary migration and recrystallization (1 Dec 2020, Colloquium)

Maurine Montagnat, Institute of Geosciences of Environment, CNRS - University of Grenoble Alpes, and Centre d'Etude de la Neige, Centre National de Recherches Météorologiques – Météo-France, CNRS, Grenoble, France: Inside a Deep Ice Core. From Small Scale Processes to Large Scale Flow (2 Dec 2020)

Atsushi Togo, National Institute for Materials Science (NIMS), Tsukuba, Japan: Tool development for phonon calculations and applications (2 Dec 2020)

Norbert Kruse, Washington State University, Pullman, WA, USA: Imaging and Chemical Probing of Catalytical Reactions with Subnanometer Resolution (7 Dec 2020)

2021

Alán Aspuru-Guzik, University of Toronto, Toronto, Canada: The Materials for Tomorrow, Today (11 Jan 2021, Colloquium)

Hosni Idrissi, Ecole Polytechnique de Louvain, Louvain-la-Neuve, Belgium: Stress Induced Grain Boundary Processes in Metals and Minerals: New Insights from *in-situ* TEM Nanomechanical Testing (14 Jan 2021)

Roland Verreet, Wire Rope Technology, Aachen, Germany: Wire Ropes and Sustainability. An Overview by the Rope Pope! (14 Jan 2021)

Markus Stricker, ICAMS, Bochum, Germany: Prismatic Slip in Magnesium (18 Jan 2021)

Yansong Shen, University of New South Wales, Sydney, Australia: Process Modeling of Reacting Flows and Industry Applications: Recent Work of Hydrogen Injection Processes in Ironmaking Blast Furnaces (21 Jan 2021)

Ben Britton, Imperial College London, UK: No Sexuality Please, We're Scientists (22 Jan 2021)

Emilio Martínez-Pañeda, Imperial College London, London, UK: Predictive Modelling of Hydrogen Assisted Fracture (18 Feb 2021)

Benoit Merle, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany: Nanoindentation at High Strain Rates: Challenges and Recent Advances (23 Feb 2021)

Johannes Schenk, Montanuniversität Leoben, Leoben, Austria: Hydrogen Meets Future Steelmaking - Applied Methods and Achieved Results for the Investigation of the Kinetics of Iron Ore Reduction with Hydrogen at Montanuniversität Leoben (24 Feb 2021, Colloquium)

Yong Zhu, North Carolina State University, Raleigh, NC, USA: MEMS-based *in-situ* Nanomechanics of Crystalline Nanowires (4 Mar 2021)

Bai-Xiang Xu, Technical University of Darmstadt, Darmstadt, Germany: Multiphysics Phase-Field Modeling and Simulation of Advanced Materials and Processing (5 Mar 2021)

Di Wan, Norwegian University of Science and Technology (NTNU), Trondheim, Norway: Hydrogen Effects on Metallic Materials Studied via Small-Scale *in-situ* Techniques (18 Mar 2021)

Shirley Meng, University of California San Diego, CA, USA: From Atom to System - How to Enable the Tera-Scale Energy Transition (25 Mar 2021, Colloquium)

Kathrin Greiff, RWTH Aachen University, Aachen, Germany: More than Recycling – Challenges & Potentials of the Circular Economy in the Case of Metals (29 Mar 2021, Colloquium)

Sho Hayakawa, University of Tennessee, Knoxville, Tennessee, USA: Active learning and on-the-fly KMC (30 Mar 2021)



Lukas Stemper, Montanuniversität Leoben, Leoben, Austria: Crossover Alloys – A New Approach for Future Aluminum Alloys (7 Apr 2021)

Fabrice Patisson, Mines Nancy, University of Lorraine, Nancy, France: Hydrogen Ironmaking: Kinetics and Modeling of the Iron Ore Reduction (8 Apr 2021)

Walid Hetaba, Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr: ChemiTEM – An Easy to Use TEM for Chemistry and Material Science (19 Apr 2021)

Varatharaja Nallathambi, Indian Institute of Technology Madras, Chennai, India: Phase Stability Studies and Evaluation of Thermal & Mechanical Properties of Entropy Stabilized Transition Metal Oxides (21 Apr 2021)

Balila Nagamani Jaya, Indian Institute of Technology (IIT) Bombay, India: Design and Applications of Length Scale Compatible Fracture Test Geometries (10 May 2021)

Maria Ibáñez, Institute of Science and Technology (IST) of Austria, Klosterneuburg, Austria: Solution-Processed Thermoelectric Materials: The Case of SnSe (10 May 2021)

Maryam Ghazisaeidi, Ohio State University, Columbus, Ohio, USA: Multi-cell Monte Carlo Method for Phase prediction (12 Mai 2021)

Rebecca Janisch, ICAMS, Bochum, Germany: Hydrogen Enhanced Decohesion at Grain Boundaries - Insights from ab-initio Calculations (27 May 2021)

Alejandro A. Franco, Université de Picardie Jules Verne, Amiens, France: Digitalization of Battery Manufacturing through Artificial Intelligence and Multiscale Modeling (01 June 2021)

Napat Vajragupta, ICAMS, Bochum, Germany: Micromechanics of Large Deformations (10 June 2021)

Rainer Abart, University of Vienna, Vienna, Austria: Growth of Mg-Aluminate Spinel at MgO-Al₂O₃ Contacts: Experiment, Nature, and Some Theory (17 June 2021)

Fadi Aldakheel, Leibniz University Hannover, Hannover, Germany: Global-Local Techniques for Adaptive Phase-Field Fracture (17 June 2021)

Philip de Goey, Eindhoven University of Technology, eindhoven, The Netherlands: Metal Energy Carriers: Renewable Fuels of the Future (30 June 2021)

Ramin Bostanabad, University of California, Irvine, CA, USA: Artificial Intelligence for Engineering Design and Computational Mechanics (6 July 2021)

Daniel Šopu, Erich Schmid Institute of Materials Science, Leoben, Austria: STZ Vortex Unit – The Key to Understand and Control Shear Banding in Metallic Glasses (6 July 2021)

Veronica Augustyn, North Carolina State University, Raleigh, NC, USA: Electrochemical Capacitance under Confinement: Implications for Electrochemical Energy Storage and Conversion (14 July 2021)

Olga Kasian, Helmholtz Zentrum Berlin, Berlin, Germany: Electrochemistry in the Renewable Energy Cycle (27 July 2021)

Leopold Lahn, Helmholtz Zentrum Berlin, Berlin, Germany: Ir based alloys for energy conversion applications (27 July 2021)

Marc Ledendecker, TH Darmstadt, Darmstadt, Germany: Design Strategies for Electrocatalyst Materials for the Oxygen Reduction Reaction (27 July 2021)

Ferdinand Biere, DeepMetis, Berlin, Germany: Be Your Own Boss – How to Found a Start Up (16 Aug 2021)

Yujiao Li, Ruhr-Universität Bochum, Bochum, Germany: Accelerated Atomic-Scale Exploration of Phase Evolution in High-Entropy Alloys (17 Aug 2021)

Fabian Sewerin, Otto von Guericke University Magdeburg, Magdeburg, Germany: Modelling the Combustion of Metal Powders in Laminar and Turbulent Flames (20 Aug 2021)

Sha Liu, IMDEA Materials Institute, Madrid, Spain: First principles prediction of Al and Mg alloys phase diagrams (24 Aug 2021)

Sergei V. Kalinin, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, USA: Realizing Physical Discovery in Imaging with Machine Learning (2 Sep 2021)

Eugen Rabkin, Department of Materials Science and Engineering, Technion, Haifa, Israel: Exploring the limits of metal strength (13 Sep 2021)

Nidhin George Mathews, Metallurgical Engineering and Materials Science Department, Indian Institute of Technology Bombay, India: Guidelines on how best to do a micro-cantilever bending based fracture test (14 Sep 2021)

Rossitza Pentcheva, Faculty of Physics, Theoretical Physics, University of Duisburg-Essen: Understanding and Improving the Catalytic Activity of Transition Metal Oxide Surfaces: Insights from DFT+U Calculations (23 Sep 2021)

Robert E. Sanders, Chongqing University, Chongqing, People's Republic of China: The Sustainability Challenge for the Aluminum Industry (30 Sep 2021)

Torsten Brezesinski, Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany: Tailoring Layered Ni-rich Oxide Cathode Materials for Solid-State Battery Applications (1 Oct 2021)

Guillaume Stechmann, ArcelorMittal Global R&D - Steel-making Process, Maizières-les-Metz, France: Machine Learning for the Steel Industry: Behind the Buzzword (5 Oct 2021)

Robert E. Sanders, Chongqing University, Chongqing, People's Republic of China: Aluminum Usage for Light Vehicles and EV's Evolution and Challenges (7 Oct 2021)



Frank Renner, Hasselt University, Belgium: Looking Deep into Li-Ion Batteries: Advanced Characterization for New Technologies (11 Oct 2021)

Robert E. Sanders, Chongqing University, Chongqing, People's Republic of China: Aluminum Alloy Aircraft Products: Performance and Manufacturing Considerations (21 Oct 2021)

Katayun Barmak, Columbia University, New York, USA: Towards a Predictive Theory of Grain Growth: Experiments and Simulations (25 Oct 2021)

Jafar Safarian, Norwegian University of Science and Technology (NTNU), Trondheim, Norway: Silicon Purification through Metallurgical Processes for PV Silicon Production (29 Oct 2021)

Andras Kovacs, Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich: What Can We Learn from Magnetic Imaging in TEM? (4 Nov 2021)

Jeffrey Bergthorson, McGill University, Montreal, Canada: Metal Fuels for Zero-Carbon Heat and Power (8 Nov 2021)

William Chueh, Stanford University, CA, USA: Designing a More Homogenous Battery: Emergent Electrochemical Phenomena at the Mesoscale (9 Nov 2021)

Katie L. Moore, University of Manchester, UK: Localisation of Hydrogen and Deuterium in Metallurgical Samples with NanoSIMS (10 Nov 2021)

Wolfgang Zeier, University of Münster & Helmholtz-Institute Münster, Germany: Understanding (Effective) Ionic Transport in Solids and Solid-state Batteries (11 Nov 2021)

Gunther Richter, Max Planck Institute for Intelligent Systems, Stuttgart: In situ Transmission Electron Microscopy Observations of Co Nanowhiskers (11 Nov 2021)

Christopher Aiden-Lee Jackson, University of Manchester, UK: What Does Race Have to Do with Science (1 Dec 2021)



Lectures and teaching at universities

2018 (not included in the Scientific Report 2016 - 2018)

Dehm, G. Transmissionselektronenmikroskopie für Fortgeschrittene. Ruhr-Universität Bochum, WS 2018/2019

Dehm, G.; Scheu, C. Atomare Charakterisierung von Werkstoffen. Heinrich-Heine Universität Düsseldorf, WS 2018/2019

Liebscher, C. Transmissionselektronenmikroskopie für Fortgeschrittene (Übung). Ruhr-Universität Bochum, WS 2018/2019

Roters, F. Prozess- und Werkstoffsimulation. RWTH Aachen, WS 2018/2019

Scheu, C. Electron Microscopy and Analytical Techniques. RWTH Aachen, WS 2018/2019

2019

Dehm, G. Mechanische Eigenschaften in kleinen Dimensionen. Ruhr-Universität Bochum, SS 2019

Dehm, G. Transmissionselektronenmikroskopie für Fortgeschrittene. Ruhr-Universität Bochum, WS 2019/2020

Hickel, T. Introduction to Quantum Mechanics in Solid-State Physics. Ruhr-Universität Bochum, WS 2019/2020

Liebscher, C. Transmissionselektronenmikroskopie für Fortgeschrittene (Übung). Ruhr-Universität Bochum, WS 2019/2020

Neugebauer, J. Application and Implementation of Electronic Structure Methods. Ruhr-Universität Bochum, WS 2019/2020

Raabe, D. Micromechanics of Materials. RWTH Aachen, SS 2019

Rohwerder, M. Surface Science and Corrosion. Ruhr-Universität Bochum, WS 2019/2020

Roters, F. Prozess- und Werkstoffsimulation. RWTH Aachen, WS 2019/2020

Scheu, C. Electron Microscopy and Analytical Techniques. RWTH Aachen, WS 2019/2020

Scheu, C. Moderne Material- und Werkstoffcharakterisierung: Vom Atom zum Bauteil. RWTH Aachen, SS 2019

Zaefferer, S. Lehrgang EBSD: Rückstreuungselektronenbeugung (EBSD) im REM. Fachhochschulzentrum (FHZ) Münster, March 2019

Zaefferer, S.; Hickel, T.; Song, W. Microstructures, Microscopy and Modelling. RWTH Aachen, SS 2019

2020

Dehm, G. Mechanische Eigenschaften in kleinen Dimensionen. Ruhr-Universität Bochum, SS 2020

Dehm, G. Transmissionselektronenmikroskopie für Fortgeschrittene. Ruhr-Universität Bochum, WS 2020/2021

Dehm, G.; Scheu, C. Atomare Charakterisierung von Werkstoffen. Heinrich-Heine Universität Düsseldorf, WS 2020/2021

Hickel, T. Introduction to Quantum Mechanics in Solid-State Physics. Ruhr-Universität Bochum, WS 2020/2021

Liebscher, C. Transmissionselektronenmikroskopie für Fortgeschrittene (Übung). Ruhr-Universität Bochum, WS 2020/2021

Neugebauer, J. Application and Implementation of Electronic Structure Methods. Ruhr-Universität Bochum, WS 2020/2021

Neugebauer, J. Electronic Structure Methods. Ruhr-Universität Bochum, SurMat T3 Module Simulations and Modelling Lecture, WS 2020/2021

Raabe, D. Micromechanics of Materials. RWTH Aachen, SS 2020

Raabe, D. Sustainable Materials Science and Green Metallurgy. RWTH Aachen, SS 2020

Rohwerder, M. IMPRS-SurMat Lecture: Corrosion. University of Duisburg-Essen and Ruhr-Universität Bochum, SS 2020

Rohwerder, M. Surface Science and Corrosion. Ruhr-Universität Bochum, WS 2020/2021

Roters, F. Prozess- und Werkstoffsimulation. RWTH Aachen, WS 2020/2021

Scheu, C. Electron Microscopy and Analytical Techniques. RWTH Aachen, WS 2020/2021

Scheu, C. Moderne Material- und Werkstoffcharakterisierung: Vom Atom zum Bauteil. RWTH Aachen, SS 2020

Springer, H. Allgemeine Werkstofftechnik. RWTH Aachen, WS 2020/2021

Zaefferer, S. Fundamentals and practical aspects of texture and microstructure measurements using EBSD-based orientation microscopy and related techniques. IIT Madras, India, Jan 2020

Zaefferer, S. Fundamentals and practical aspects of texture and microstructure measurements using EBSD-based orientation microscopy and related techniques. MPIE Düsseldorf, Feb and Mar 2020

Zaefferer, S.; Hickel, T.; Song, W. Microstructures, Microscopy and Modelling. RWTH Aachen, SS 2020

2021

Dehm, G. Mechanische Eigenschaften in kleinen Dimensionen. Ruhr-Universität Bochum, SS 2021

Dehm, G. Transmissionselektronenmikroskopie für Fortgeschrittene. Ruhr-Universität Bochum, WS 2021/2022

El-Zoka, A. Introduction to Atom Probe Tomography. MPIE Düsseldorf, IMPRS-SurMat, Aug 2021

Gault, B. Graduate course on Atom Probe Tomography, as part of the Centre for Doctoral Training on Materials Characterisation. Imperial College London, UK, SS 2021

Liebscher, C. Transmissionselektronenmikroskopie für Fortgeschrittene (Übung). Ruhr-Universität Bochum, WS 2021/2022

Raabe, D.; Cojocaru-Mirédin, O.; El-Zoka, A.; Kontis, P.; Ma, Y.; Mianroodi, J. R.; Ponge, D.; Souza Filho, I. R.; Sandlöbes-Haut, S.; Zaefferer, S.; Zhao, H. Sustainable Materials Science and Green Metallurgy (Sustainable Materials and Metallurgical Science & Engineering). RWTH Aachen, SS 2021

Rohwerder, M. Surface Science and Corrosion. Ruhr-Universität Bochum, WS 2021/2022

Scheu, C. Advanced Characterisation. RWTH Aachen, WS 2021/2022

Scheu, C. Moderne Material- und Werkstoffcharakterisierung: Vom Atom zum Bauteil. RWTH Aachen, SS 2021

Springer, H. Allgemeine Werkstofftechnik. RWTH Aachen, WS 2021/2022

Zaefferer, S.; Hickel, T.; Song, W. Microstructures, Microscopy and Modelling. RWTH Aachen, SS 2021

Zaefferer, S.; Motaman, S. A. H. Metallic Materials (Microstructure, Microscopy, Modelling). RWTH Aachen, SS 2021

Invited talks at conferences and colloquia

2018 (not included in Scientific Report 2016 - 2018)

Dehm, G.: *Defects in alloys: New insights by advanced in-situ electron microscopy* (Symposium Netzwerk Elektronenmikroskopie: Struktur und Chemie an Werkstoffen und biologischen Systemen, Naturwissenschaftliches und Medizinisches Institut an der Universität Tübingen. Reutlingen, Germany. 12 Nov. 2018)

Garzón-Manjón, A.: *Controlling the structure and composition of multinary alloy nanoparticles for energy applications* (Leitat Institut Colloquium. Barcelona, Spain. 30 Nov. 2018)

Kürnstener, P.; Wilms, M. B.; Weisheit, A.; Bajaj, P.; Li, X.; Leinenbach, C.; Jäggle, E. A.; Raabe, D.: *Process and Alloy Design for In-Situ Precipitation Strengthening of Al-Sc Alloys During Laser Metal Deposition* (Metal Additive Manufacturing Conference. Vienna, Austria. 21 Nov. 2018)

Kürnstener, P.; Wilms, M. B.; Weisheit, A.; Barriobero-Vila, P.; Jäggle, E. A.; Raabe, D.: *Designing a novel Fe-Ni-Al-Ti Maraging steel tailor-made for Laser Metal Deposition* (Metal Additive Manufacturing Conference. Vienna, Austria. 21 Nov. 2018)

Kürnstener, P.; Wilms, M. B.; Weisheit, A.; Barriobero-Vila, P.; Jäggle, E. A.; Raabe, D.: *Designing Fe-Ni-Al and Fe-Ni-Ti Maraging steels tailor-made for Laser Metal Deposition by exploiting Intrinsic Heat Treatment* (Alloys for Additive Manufacturing Symposium. Sheffield, UK. 03 Sep. 2018)

Li, Z.; Su, J.; Lu, W.; Wang, Z.; Raabe, D.: *Metastable high-entropy alloys: design, structure and properties* (2nd International Conference on High-Entropy Materials (ICHEM 2018). Jeju, South Korea. 09 Dec. 2018)

Liebscher, C.; Peter, N. J.; Meiners, T.; Frolov, T.; Dehm, G.: *Atomic scale observations of grain boundary phase transformations* (Materials Science and Engineering Congress 2018. Darmstadt, Germany. 26 Sep. 2018)

Raabe, D.; Kwiatkowski da Silva, A.; Ponge, D.; Li, Z.; Makineni, S. K.; Li, L.; Gault, B.: *Grain boundary segregation and transformation in complex alloys* (Fall Meeting. Boston, MA, USA. 25 Nov. 2018)

Raabe, D.; Lu, W.; Ponge, D.; Li, Z.; Kwiatkowski da Silva, A.; Makineni, S. K.; Kontis, P.; Wu, X.; Gault, B.: *Local and global alloy design: metastability of single lattice defects and alloys with extreme metastability* (MIT Workshop on Alloy Design. Cambridge, MA, USA. 30 Nov. 2018)

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Makineni, S. K.; Peng, Z.; Li, L.; Kontis, P.; Wu, X.; Springer, H.; Belde, M. M.; Gault, B.: *Segregation and Transformation at Lattice Defects in Complex Alloys: A Microstructure Design Toolbox* (MRS Fall Meeting. Boston, MA, USA. 25 Nov. 2018)

Scheu, C.; Hengge, K. A.: *Unravelling catalyst growth and degradation mechanisms via STEM* (International Workshop on Advanced and In-situ Microscopies of Functional Nanomaterials and Devices, IAMNano 2018. Hamburg, Germany. 14 Oct. 2018)

Seol, J. B.; Ko, W.-S.; Bae, J. W.; Jo, Y. H.; Li, Z.; Choi, P.-P.; Raabe, D.; Kim, H. S.: *Transition in boron boundary cohesion from effectiveness to harmfulness with respect to application temperatures: high-entropy alloys and Ni-based superalloys* (2nd International Conference on High-Entropy Materials (ICHEM 2018). Jeju, South Korea. 09 Dec. 2018)

Stephenson, L.: *Advanced quantitative analysis for Atom Probe Tomography* (APT school at Groupe de Physique des Matériaux (GPM), Université de Rouen. Saint Etienne du Rouvray, France. 18 Oct. 2018)

Stephenson, L.; Rusitzka, A. K.; Gault, B.: *Seeing atoms in biological materials: a new frontier for atomic-scale tomography* (Volkswagen Stiftung Symposium. Bremen, Germany. 31 Oct. 2018)

Sun, B.; Ponge, D.; Fazeli, F.; Scott, C.; Yue, S.; Raabe, D.: *Revealing fracture mechanisms of medium manganese steels with and without delta-ferrite* (6th International Conference on Advanced Steels (ICAS 2018). Jeju, South Korea. 18 Nov. 2018)

Todorova, M.; Yoo, S.-H.; Surendralal, S.; Neugebauer, J.: *Ab initio modelling of solid/liquid interfaces: Challenges and insights* (DESY Seminar. Hamburg, Germany. 20 Oct. 2018)

Zaefferer, S.: *The importance of microstructures for the energy conversion efficiency of materials for photovoltaic and photothermic applications* (Development of Photovoltaic Solar Energy in Africa by the Year 2030. Abidjan, Republik Côte d'Ivoire. 08 Nov. 2018)

2019

Abdellaoui, L.; Zhang, S.; Rodenkirchen, C.; Zaefferer, S.; Bueno Villoro, R.; Guen, E.; Chapuis, P.-O.; Gomès, S.; Cojocar-Mirédin, O.; Yu, Y.; Amouyal, Y.; Raabe, D.; Snyder, G. J.; Scheu, C.: *Correlation of Microstructures and Thermal Conductivity of the Thermoelectric Material $Ag_{16.7}Sb_{30}Te_{53.3}$* (North American Thermoelectric workshop, Northwestern University. Evanston, Chicago, IL, USA. 30 Aug. 2019)

Abdellaoui, L.; Zhang, S.; Rodenkirchen, C.; Zaefferer, S.; Bueno Villoro, R.; Guen, E.; Chapuis, P.-O.; Gomès, S.; Cojocar-Mirédin, O.; Yu, Y.; Amouyal, Y.; Raabe, D.; Snyder, G. J.; Scheu, C.: *Effect of planar defects on the thermal conductivity of $Ag_{16.7}Sb_{30}Te_{53.3}$ bulk thermoelectric* (6th German/Korean Thermoelectric workshop. Daegu, South Korea. 05 Jul. 2019)

Brinckmann, S.; Dehm, G.: *Severe deformation of a lamellar microstructure: pearlitic steel as a case study* (TMS 2019. San Antonio, TX, USA. 10 Mar. 2019)

Dehm, G.: *Do we understand the microstructure and properties of materials: New insights by advanced microscopy techniques* (Metallurgical Engineering and Materials Science Department, Indian Institute of Technology. Mumbai, India. 15 Jul. 2019)

Dehm, G.: *Können hohe Festigkeit und Zähigkeit in Verschleißschutzschichten kombiniert werden? Eine grundlegende Untersuchung an Mo₂BC* (12. Tagung Gefüge und Bruch. Bochum, Germany. 13 Feb. 2019)

Dehm, G.: *Können hohe Festigkeit und Zähigkeit in Verschleißschutzschichten kombiniert werden? Eine grundlegende Untersuchung an Mo₂BC* (12. Tagung Gefüge und Bruch. Bochum, Germany. 13 Feb. 2019)

Dehm, G.: *Micro- and Nanomechanical Testing of Materials - From Materials Physics to Materials Design* (Convegno Nazionale INSTM XII. Ischia Porto, Italy. 21 Jul. 2019)

Dehm, G.: *Probing the mechanics of dislocation - grain boundary interactions: Lessons learned from in situ micro-compression experiments* (14th International Conference on Local Mechanical Properties 2019 (plenary). Prague, Czech Republic. 06 Nov. 2019)

Dehm, G.: *Resolving grain boundary phase transformations by advanced STEM for fcc metals and multinary alloys* (6th International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM-2019). Chennai, India. 08 Jul. 2019)

Dehm, G.: *Towards understanding dislocation-based plasticity in high entropy alloys by in-situ TEM* (Spring Meeting of the German Physical Society (DPG). Regensburg, Germany. 01 Apr. 2019)

Diehl, M.; Cereceda, D.; Marian, J.; Liu, C.; Dong, J.; Wicke, M.; Brückner-Foit, A.; Kamachali, R. D.; Shanthraj, P.; Roters, F.; Eisenlohr, P.; Raabe, D.: *Coupling Crystal Plasticity and Phase Field Methods - The Future of Integrated Computational Materials Engineering?* (Recent Advances in the Modeling and Simulation of the Mechanics of Nanoscale Materials. Philadelphia, PA, USA. 23 Aug. 2019)

Diehl, M.; Cereceda, D.; Marian, J.; Liu, C.; Dong, J.; Wicke, M.; Brückner-Foit, A.; Kamachali, R. D.; Shanthraj, P.; Roters, F.; Eisenlohr, P.; Raabe, D.: *DAMASK: The Düsseldorf Advanced Materials Simulation Kit* (Seminar of the Department of Materials Science and Engineering of the Ohio State University. Columbus, OH, USA. 26 Aug. 2019)

Diehl, M.; Kühbach, M.; Kertsch, L.; Traka, K.; Raabe, D.: *Coupled Experimental-Computational Analysis of Primary Static Recrystallization in Low Carbon Steel* (Seminar of the Department of Mechanical Science and Engineering of the University of Illinois. Urbana-Champaign, IL, USA. 27 Sep. 2019)

Diehl, M.; Shanthraj, P.; Eisenlohr, P.; Roters, F.; Raabe, D.: *Beyond Crystal Plasticity - Developing Tools for Integrated Computational Materials Engineering* (Seminar of the Tسان Group, MIT. Boston, MA, USA. 19 Jul. 2019)

Duarte, M. J.; Fang, X.; Rao, J.; Brinckmann, S.; Dehm, G.: *Hydrogen-metal interactions by in-situ and ex-situ nanoindentation* (2nd LINCET Symposium, Downing College. Cambridge, UK. 05 Apr. 2019)

El-Zoka, A.; Langelier, B.; Newman, R. C.: *Characterization and Functional Improvement of Nanoporous Metals* (236th ECS Meeting. Atlanta, GA, USA. 13 Oct. 2019)

Freysoldt, C.: *Concepts and algorithms in SPHInX* (Weierstraß-Institut für Angewandte Analysis und Stochastik, Online Seminar. Berlin, Germany. 09 May 2019)

Freysoldt, C.: *Concepts and algorithms in SPHInX* (Weierstraß-Institut für Angewandte Analysis und Stochastik, Invited Seminar. Berlin, Germany. 09 May 2019)

Freysoldt, C.: *Modelling of charged point defects with density-functional theory* (4th International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices, National Institute for Fusion Science (NIFS). Toki, Japan. 18 Jun. 2019)

Garzón-Manjón, A.; Meyer, H.; Grochla, D.; Löffler, T.; Savan, A.; Schuhmann, W.; Ludwig, A.; Scheu, C.: *Pathways for fabrication of amorphous and crystalline multinary nanoparticles for electrocatalyst* (14th International Conference on Materials Chemistry MC14. Birmingham, UK. 08 Jul. 2019)

Gault, B.: *A not-so-brief introduction to atom probe tomography: from fundamentals to atomic-scale insights into engineering materials* (Seminar, Imperial College London. London, UK. 19 Feb. 2019)

Gault, B.: *An introduction to atom probe tomography: from fundamentals to atomic-scale insights into engineering materials* (Seminar, University of British Columbia. Vancouver, BC, Canada. 24 May 2019)

Gault, B.: *An introduction to atom probe tomography: from fundamentals to atomic-scale insights into engineering materials* (Seminar, University of Manchester. Manchester, UK. 24 Jun. 2019)

Gault, B.: *An introduction to atom probe tomography: from fundamentals to atomic-scale insights into engineering materials* (Rolls Royce Lunch Time Seminar. Derby, UK. 01 Jul. 2019)

Gault, B.: *Atom Probe Tomography to help Understand Deformation Mechanisms in Metallic Alloys* (The International Conference on Metallurgical Coatings and Thin Films 2019. San Diego, CA, USA. 19 May 2019)

Gault, B.: *Can machine learning bring atom probe microscopy closer to analytical atomic-scale tomography* (12th International Symposium on Atomic Level Characterizations for New Materials and Devices (ALC 19). Kyoto, Japan. 20 Oct. 2019)

Gault, B.: *Quantifying hydrogen by atom probe tomography* (Seminar, Oxford University. Oxford, UK. 25 Jun. 2019)

Gault, B.: *Some kind of introduction to atom probe tomography* (Annual Meeting of the Canadian Society for Microscopy. Vancouver, BC, Canada. 22 May 2019)



- Gault, B.; Breen, A. J.; Mouton, I.; Lu, W.; Wang, S.; Szczepaniak, A.; Kontis, P.; Stephenson, L.; Kwiatkowski da Silva, A.; Liebscher, C.; Herbig, M.; Raabe, D.; Britton, T. B.: *Atomic scale analysis of grain boundary deuteride growth front in Zircaloy-4* (TMS 2019. San Antonio, TX, USA. 10 Mar. 2019)
- Gault, B.; Makineni, S. K.; He, J.; Lenz, M.; Neumeier, S.; Spiecker, E.; Raabe, D.: *Solute segregation effect at planar defects during creep of CoNi- & Co-based superalloys* (TMS 2019. San Antonio, TX, USA. 10 Mar. 2019)
- Han, F.; Diehl, M.; Roters, F.; Raabe, D.: *Multi-scale modeling of plasticity* (ICIAM 2019 - The 9th International Congress on Industrial and Applied Mathematics. Valencia, Spain. 15 Jul. 2019)
- Herbig, M.: *Joint Nanoscale Structural and Chemical Characterization by Correlative Atom Probe Tomography and Transmission Electron Microscopy* (Joint Workshop on Nano-Characterisation (4TU.HTM / M2i). Utrecht, The Netherlands. 28 Oct. 2019)
- Hickel, T.: *Application of Density Functional Theory in the Context of Phase Diagram Modelling* (MSIT Winter School on Materials Chemistry. Castle Ringberg, Tegernsee. 03 Mar. 2019)
- Hickel, T.; Dey, P.; McEniry, E.; Yao, M.; Herbig, M.; Lipińska-Chwałek, M.; Liebscher, C.; Mušić, D.; Hallstedt, B.; Haase, C.; Song, W.; Scheu, C.; Ponge, D.; Raabe, D.; Neugebauer, J.: *κ carbide microstructures and the role of interfaces in high-Mn lightweight steels* (High-Mn Steel 2019. Aachen, Germany. 31 Mar. 2019)
- Hickel, T.; Dutta, B.; Stockem, I.; Körmann, F.; Neugebauer, J.: *Ab initio design strategies for NiMn-based FSMA* (6th Int. Conf. of Ferromagnetic Shape-Memory Alloys CFMSA. Prague, Czech Republic. 02 Jun. 2019)
- Hickel, T.; Gupta, A.; Neugebauer, J.; Kavakbasi, B. T.; Buranova, Y.; Kulitskiy, V. A.; Wilde, G.; Divinski, S. V.: *Precipitate-induced nonlinearities of solute diffusion in Al-based alloys* (15th Diffusion in Solids and Liquids (DSL) Conference. Athens, Greece. 27 Jun. 2019)
- Hickel, T.; Janßen, J.; Sözen, H. I.; Körmann, F.; Neugebauer, J.; Lysogorskiy, Y.; Drautz, R.: *Ab initio simulation of finite temperature phase stabilities: Concepts and application* (HetSys Launch Event. Warwick, UK. 09 Sep. 2019)
- Hickel, T.; Janßen, J.; Sözen, H. I.; Körmann, F.; Surendralal, S.; Todorova, M.; Lysogorskiy, Y.; Drautz, R.; Neugebauer, J.: *High-throughput optimization of finite temperature phase stabilities: Concepts and application* (Spring Meeting of the German Physical Society (DPG). Regensburg, Germany. 4 Apr. 2019)
- Hickel, T.; Zendegani, A.; Körmann, F.; Neugebauer, J.: *Energetics of non-stoichiometric stacking faults in Fe-Nb alloys: An ab initio study* (TMS 2019. San Antonio, TX, USA. 10 Mar. 2019)
- Huber, L.; Hadian, R.; Grabowski, B.; Neugebauer, J.: *Computing and modelling solute-grain boundary interaction* (Canadian Materials Science Conference. Vancouver, Canada. 12 Jun. 2019)
- Ikeda, Y.; Körmann, F.; Neugebauer, J.: *Impact of Interstitial Alloying of High Entropy Alloys from First Principles* (2019. San Antonio, TX, USA. 10 Mar. 2019)
- Janßen, J.; Hickel, T.; Neugebauer, J.: *Automated ab-initio Determination of Materials Properties at finite Temperatures with pyiron* (CNLS Seminar. Los Alamos, NM, USA. 10 Dec. 2019)
- Jeong, J.: *Advanced transmission electron microscopy of nanomaterials using In-situ TEM and precession electron diffraction* (Seminar, Korea Institute of Science and Technology (KIST). Seoul, South Korea. 04 Nov. 2019)
- Jeong, J.: *Advanced transmission electron microscopy of nanomaterials using In-situ TEM and precession electron diffraction* (Seminar, Korea Institute of Materials Science (KIMS). Seoul, South Korea. 08 Nov. 2019)
- Jeong, J.: *Advanced transmission electron microscopy of nanomaterials using In-situ TEM and precession electron diffraction* (Seminar, Korea Institute of Industrial Technology (KITECH). Seoul, South Korea. 13 Nov. 2019)
- Jeong, J.; Kim, J.; Kiener, D.; Oh, S. H.: *In-situ TEM observation of twin-dominated deformation of Mg single crystals* (KSM Annual Fall Conference 2019. Gyeongju, South Korea. 14 Nov. 2019)
- Kontis, P.; Liliensten, L.; Kürnstener, P.; Cervellon, A.; Cormier, J.; Raabe, D.; Gault, B.: *The effect of segregation of solutes at crystal defects on the mechanical performance of superalloys* (10th Pacific Rim International Conference on Advance Materials and Processing (PRICM-10). Xi'an, China. 18 Aug. 2019)
- Kontis, P.; Makineni, S. K.; Wu, X.; Mianroodi, J. R.; Shanthraj, P.; Cormier, J.; Raabe, D.; Gault, B.: *Understanding deformation mechanisms in superalloys through atomic scale microanalysis* (TMS 2019. San Antonio, TX, USA. 10 Mar. 2019)
- Körmann, F.; Ikeda, Y.; Srinivasan, P.; Neugebauer, J.; Grabowski, B.; Kostichenko, T.; Shapeev, A.: *Phase stability and mechanical properties of high entropy and chemically complex alloys* (MS&T Annual Meeting. Portland, OR, USA. 01 Oct. 2019)
- Kürnstener, P.; Hariharan, A.; Jung, H. Y.; Peter, N. J.; Wilms, M. B.; Weisheit, A.; Barriobero-Vila, P.; Gault, B.; Raabe, D.; Jäggle, E. A.: *Application of Atom Probe Tomography to Complex Microstructures of Laser Additively Manufactured Samples* (Microscopy & Microanalysis Conference. Portland, OR, USA. 04 Aug. 2019)
- Li, Z.; Su, J.; Lu, W.; Luo, H.; Wang, Z.; Wu, X.; Raabe, D.: *Recent progresses in the understanding of metastable high-entropy alloys* (TMS 2019. San Antonio, TX, USA. 10 Mar. 2019)
- Liebscher, C.: *Transmission electron microscopy - Characterization across the length scales* (Pre-conference workshop of the 26th International Symposium on Metastable, Amorphous and Nanostructured Materials 2019 (ISMANAM 2019). Chennai, India. 07 Jul. 2019)

Liebscher, C.; Meiners, T.; Harzer, T. P.; Freysoldt, C.; Dehm, G.: *Atomic scale phase separation tendencies in nanostructured copper alloys* (26th International Symposium on Metastable, Amorphous and Nanostructured Materials 2019 (ISMANAM 2019). Chennai, India. 08 Jul. 2019)

Liebscher, C.; Meiners, T.; Peter, N. J.; Frolov, T.; Dehm, G.: *Experimental discovery of grain boundary phase transformations unveiled by atomistic simulations* (PICS³ 2019 Meeting, Centre Interdisciplinaire de Nanoscience de Marseille. Marseille, France. 21 Jun. 2019)

Liebscher, C.; Meiners, T.; Peter, N. J.; Frolov, T.; Dehm, G.: *Experimental discovery of grain boundary phase transformations unveiled by atomistic simulations* (Colloquium of IIT Gandhinagar. Palaj, India. 05 Jul. 2019)

Liebscher, C.; Meiners, T.; Peter, N. J.; Frolov, T.; Dehm, G.: *Exploration of interfacial transitions by correlating atomic scale microscopy with atomistic simulations* (TMS 2019. San Antonio, TX, USA. 10 Mar. 2019)

Liebscher, C.; Stoffers, A.; Alam, M.; Lymperakis, L.; Cojocaru-Mirédin, O.; Gault, B.; Neugebauer, J.; Dehm, G.; Scheu, C.; Raabe, D.: *Asymmetric Line Segregation at Faceted Si Grain Boundaries* (TMS 2019. San Antonio, TX, USA. 10 Mar. 2019)

Liebscher, C.; Stoffers, A.; Alam, M.; Lymperakis, L.; Cojocaru-Mirédin, O.; Gault, B.; Neugebauer, J.; Scheu, C.; Raabe, D.; Meiners, T.; Frolov, T.; Dehm, G.: *How do grain boundaries transform on the atomic level?* (International Workshop on Advanced and In-situ Microscopies of Functional Nanomaterials and Devices, IAMNano 2019. Düsseldorf, Germany. 29 Oct. 2019)

Lim, J.; Kim, S.-H.; Sahu, R.; Aymerich Armengol, R.; Kasian, O.; Choi, P.-P.; Stephenson, L.; Gault, B.; Scheu, C.: *Detection of trace impurities and other defects in functional nanomaterials* (International Workshop on Advanced and In-situ Microscopies of Functional Nanomaterials and Devices, IAMNano 2019. Düsseldorf, Germany. 27 Oct. 2019)

Liu, C.; Garner, A.; Zhao, H.; Gault, B.; Prangnell, P.; Raabe, D.; Shanthraj, P.: *CALPHAD-informed phase-field modeling of grain boundary microchemistry and microstructure in Al-Zn-Mg-Cu alloys* (LightMAT 2019 - 3rd Conference & Exhibition on Light Materials. Manchester, UK. 05 Nov. 2019)

Lymperakis, L.: *Surface rehybridization and strain effects on the composition and the properties of ternary III Nitride alloys* (19th International Conference on Crystal Growth and Epitaxy. Keystone, CO, USA. 28 Jul. 2019)

Lymperakis, L.: *Surface rehybridization effects of B incorporation at GaN and AlN surfaces: A potential route to overcome bulk solubility limits* (4th International Workshop on Ultraviolet Materials and Devices. Saint Petersburg, Russia. 08 Sep. 2019)

Lymperakis, L.: *Ab-initio based investigations of surface reconstructions and strain effects on the compositional limits of ternary III-Nitride alloys* (National Institute of

Advanced Industrial Science and Technology (AIST) Colloquium. Tsukuba, Japan. 09 Oct. 2019)

Lymperakis, L.: *Ab-initio based description and design of nitride surfaces: The role of surface rehybridization on alloy composition and ordering* (Materials Research Meeting 2019 (Materials Research Society of Japan). Yokohama, Japan. 10 Oct. 2019)

Mendive-Tapia, E.: *Ab-initio Free energy of antiferromagnetic phases: a hierarchy of local moment correlation functions* (Current Research in Magnetism (CRIM) 2019: Recent advances in Antiferromagnetism. London, UK. 18 Sep. 2019)

Nandy, S.; Zaefferer, S.: *On the role of Ca, Zn and Al for ductilization of Mg alloys* (27th International Conference on Materials and Technology (27 ICM&T). Portoroz, Slovenia. 16 Oct. 2019)

Neugebauer, J.; Surendralal, S.; Todorova, M.: *Extending First-Principles Calculations to Model Electrochemical Reactions at the Solid-Liquid Interface* (Towards Reality in Nanoscale Materials X. Levi, Finland. 12 Feb. 2019)

Neugebauer, J.; Janßen, J.; Körmann, F.; Hickel, T.; Grabowski, B.: *Exploiting large ab initio data spaces to design materials* (Opening of Christian Doppler Laboratory for nanoscale phase transformations. Linz, Austria. 28 Feb. 2019)

Neugebauer, J.; Todorova, M.; Grabowski, B.; Hickel, T.: *Modelling structural materials in realistic environments by ab initio thermodynamics* (Hume-Rothery Award Symposium, TMS 2019. San Antonio, TX, USA. 13 Mar. 2019)

Neugebauer, J.: *Automizing work flows in computational materials design* (Traceability and securing of results as essential challenges of research in the digital age. Berlin, Germany. 09 Apr. 2019)

Neugebauer, J.; Janßen, J.; Körmann, F.; Hickel, T.; Grabowski, B.: *Exploiting large ab initio data spaces to design materials with superior mechanical properties* (2019 BIOVIA User Conference. Düsseldorf, Germany. 15 May 2019)

Neugebauer, J.; Janßen, J.; Hickel, T.: *Automated uncertainty analysis and quantification for high-precision DFT calculations* (Workshop "Precision Quantification in DFT." Louvaine-la-Neuve, Belgien. 23 May 2019)

Neugebauer, J.: *Machine Learning in Materials: Screening and Discovery* (Gordon Research Conference Physical Metallurgy „Coupling Computation, Data Science and Experiments in Physical Metallurgy“. Manchester, NH, USA. 08 Jul. 2019)

Neugebauer, J.; Huber, L.; Körmann, F.; Grabowski, B.; Hickel, T.: *Ab initio input for multiphysics models: Accuracy, performance and challenges* (ISAM4: The fourth International Symposium on Atomistic and Multiscale Modeling of Mechanics and Multiphysics. Erlangen, Germany. 05 Aug. 2019)



Neugebauer, J.: *Ab initio guided materials design and discovery* (Inaugural Symposium for Computational Materials, Skoltech. Moscow, Russia. 04 Sep. 2019)

Neugebauer, J.; Stockem, I.; Hegde, O.; Freysoldt, C.; Körmann, F.; Hickel, T.; Alling, B.: *Ab initio description of coupling phenomena between magnetic and structural degrees of freedom* (EASTMAG2019 – VII Euro-Asian Symposium "Trends in Magnetism." Jekaterinburg, Russia. 10 Sep. 2019)

Neugebauer, J.; Janßen, J.; Körmann, F.; Hickel, T.; Grabowski, B.: *Ab initio descriptors to design materials with superior mechanical properties* (Materials Day, ETH Zürich. Zürich, Switzerland. 20 Nov. 2019)

Neugebauer, J.: *Machine Learning in Materials: Screening and Discovery* (National Institute of Advanced Industrial Science and Technology (AIST). Tsukuba, Japan. 09 Dec. 2019)

Neugebauer, J.; Janßen, J.; Huber, L.; Körmann, F.; Hickel, T.; Grabowski, B.: *Construction and exploitation of large ab initio data spaces to design materials with superior mechanical properties* (MRS-J 2019. Yokohama, Japan. 11 Dec. 2019)

Neugebauer, J.; Janßen, J.; Körmann, F.; Hickel, T.; Grabowski, B.: *Exploration of large ab initio data spaces to design materials with superior mechanical properties* (Physics and Theoretical Division Colloquium. Los Alamos, NM, USA. 31 Jan. 2019)

Neugebauer, J.; Surendralal, S.; Todorova, M.: *First-principles approach to model electrochemical reactions at solid-liquid interfaces* (ACS 2019 Fall Meeting & Exhibition. San Diego, CA, USA. 25 Aug. 2019)

Peter, N. J.; Meiners, T.; Duarte, M. J.; Kirchlechner, C.; Frolov, T.; Liebscher, C.; Dehm, G.: *Grain boundary phase transformations in Cu: New insights by advanced STEM* (65. Metallkunde-Kolloquium. Lech am Arlberg, Austria. 23 Apr. 2019)

Raabe, D.: *Atomic-Scale Analysis of Chemistry at Lattice Defects* (The KAIST Lecture in Materials Science and Engineering 2019, Korea Advanced Institute of Science and Technology KAIST. Daejeon, Korea. 07 May 2019)

Raabe, D.: *Compositional Lattice Defect Manipulation for Microstructure Design* (The Bauerman Lecture 2019, Department of Materials, Imperial College London, Royal School of Mines. London, UK. 28 Feb. 2019)

Raabe, D.: *Metastable Nanostructured Metallic Alloy* (The KAIST Lecture in Materials Science and Engineering 2019, Korea Advanced Institute of Science and Technology KAIST. Daejeon, Korea. 07 May 2019)

Raabe, D.; Katnagallu, S.; Stephenson, L.; Balachandran, S.; Freysoldt, C.; Neugebauer, J.; Gault, B.: *Imaging single vacancies and atoms using joint FIM and APT experiments* (Conference on Possibilities and Limitations of Quantitative Materials Modeling and Characterization. Bernkastel-Kues, Germany. 20 May 2019)

Raabe, D.; Neugebauer, J.; Körmann, F.; Rao, Z.; Gault, B.; Lu, W.; Li, Z.: *Metastability High Entropy Alloy Design* (MRS Fall Meeting. Boston, MA, USA. 01 Dec. 2019)

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Katnagallu, S.; Stephenson, L.; Freysoldt, C.; Diehl, M.; Liebscher, C.; Kamachali, R. D.; Zaefferer, S.; Neugebauer, J.; Sandlöbes, S.; Gault, B.; Scheu, C.; Roters, F.: *From Atomistic Understanding to Engineering Design of Advanced Medium and High Manganese Steels* (4th International Conference on medium and high Manganese steels. Aachen, Germany. 01 Apr. 2019)

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Makineni, S. K.; Katnagallu, S.; Stephenson, L.; Freysoldt, C.; Neugebauer, J.; Gault, B.: *Chemistry and Structure of Lattice Defects* (Physics Colloquium, Faculty of Physics, University Duisburg-Essen. Duisburg, Germany. 15 May 2019)

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Makineni, S. K.; Katnagallu, S.; Stephenson, L.; Kontis, P.; Freysoldt, C.; Neugebauer, J.; Gault, B.: *Chemistry at Lattice Defects Probed at Atomic Scale* (20th International Union of Materials Research Societies International Conference in Asia IUMRS. Perth, Australia. 22 Sep. 2019)

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Makineni, S. K.; Katnagallu, S.; Stephenson, L.; Kontis, P.; Wu, X.; Freysoldt, C.; Neugebauer, J.; Gault, B.: *Chemistry at Lattice Defects Probed at Atomic Scale* (The 53rd Annual Meeting of the Israel Society for Microscopy, Tel Aviv, Israel. Tel Aviv, Israel. 29 May 2019)

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Makineni, S. K.; Katnagallu, S.; Stephenson, L.; Kontis, P.; Wu, X.; Freysoldt, C.; Neugebauer, J.; Gault, B.: *Interaction of Chemistry and Structure at Lattice Defects at Atomic Scale* (Russell Berrie Nanotechnology Institute, Technion, Haifa, Israel. Haifa, Israel. 28 May 2019)

Raabe, D.; Ponge, D.; Li, Z.; Neugebauer, J.; Körmann, F.; Rao, Z.; Gault, B.: *Metastable High Entropy Alloys* (World Congress on High Entropy Alloys. Seattle, WA, USA. 18 Sep. 2019)

Rohwerder, M.: *Die Kelvinsondentechnik in der Korrosion: von der Grundlagenforschung bis hin zu potentiellen Anwendungen im Feld* (ProcessNet Meeting "Elektrochemische Prozesse", Dechema-Haus. Frankfurt, Germany. 21 Jan. 2019)

Rohwerder, M.: *Hydrogen embrittlement, hydrogen traps, high sensitive detection of hydrogen with high spatial resolution, corrosion* (Dreiländerkorrosionstagung, Dechema-Haus. Frankfurt, Germany. 09 Apr. 2019)

Rohwerder, M.: *Intelligent coatings for corrosion protection: on the need for new coating concepts* (International Conference on Corrosion Protection and Application (ICCPA 2019). Chongqing, China. 10 Oct. 2019)

Rohwerder, M.: *Scanning Kelvin Probe based techniques for mapping hydrogen distribution in metals and their application for investigating hydrogen embrittlement* (Workshop "Hydrogen in Metals", St Anne's College. Oxford, UK. 15 Apr. 2019)

- Rohwerder, M.: *Zinc alloy coatings and nano-composite coatings for corrosion protection: From the basics to new challenges* (IIM NMD ATM 2019: Advanced Materials for Industrial and Societal Applications. Kovalam, Thiruvananthapuram, India. 13 Nov. 2019)
- Roters, F.: *DAMASK - The Düsseldorf Advanced Material Simulation Kit for studying multi-physics crystal plasticity phenomena* (TOOLKIT Seminar Integrated Computational Materials Engineering, OCAS. Gent, Belgium. 09 Jul. 2019)
- Roters, F.; Han, F.: *Calibrating yield surface models based on full yield crystal plasticity simulations* (M2i conference "Meeting Materials." Noordwijkerhout, The Netherlands. 10 Dec. 2019)
- Scheu, C.: *Advanced Cs corrected STEM imaging coupled to 3D atom probe tomography* (SCANDEM 2019. Gothenburg, Sweden. 12 Jun. 2019)
- Scheu, C.: *Materials for renewable energy applications* (Metallurgical Engineering and Materials Science Department Colloquium, Indian Institute of Technology. Mumbai, India. 15 Jul. 2019)
- Scheu, C.; Folger, A.: *Annealing treatment in various atmospheres: A tool to control structure and properties of TiO₂ nanowires* (6th International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMA-NAM-2019). Chennai, India. 08 Jul. 2019)
- Scheu, C.; Hieke, S. W.: *Fundamentals and Applications of Electron Energy-Loss Spectroscopy in a Scanning Transmission Electron Microscope* (Universita' Roma Tre Colloquium. Roma, Italy. 25 Jul. 2019)
- Scheu, C.; Hieke, S. W.: *How stable are thin Aluminium films: Dewetting phenomena observed by in-situ electron microscopy* (Microscopy Conference 2019 (MC2019). Berlin, Germany. 01 Sep. 2019)
- Scheu, C.; Zhang, S.: *Effect of interfaces on the photoelectrochemical performance of functional oxides* (PICS³ 2019 Meeting, Centre Interdisciplinaire de Nanoscience de Marseille. Marseille, France. 21 Jun. 2019)
- Shah, V.; Diehl, M.; Roters, F.: *Prediction of Nucleation Sites for Recrystallization using Crystal Plasticity Simulations* (7th International Conference on Recrystallization and Grain Growth. Ghent, Belgium. 04 Aug. 2019)
- Stein, F.: *Experimental Determination of Phase Diagrams* (3rd MSIT Winter School on Materials Chemistry. Castle Ringberg, Tegernsee. 04 Mar. 2019)
- Stein, F.: *Fe-Al-based Materials: Phase Diagrams, Properties, and Potential for Applications* (Seminar, Hokkaido University of Science. Sapporo, Japan. 28 Oct. 2019)
- Stein, F.: *Stability Competition between Laves Phase Polytypes* (Tokyo Institute of Technology. Tokyo, Japan. 01 Nov. 2019)
- Stein, F.: *The Co-Ti system revisited: About the cubic-to-hexagonal Laves phase transformation and other controversial features of the phase diagram* (Seminar, Hokkaido University. Sapporo, Japan. 29 Oct. 2019)
- Stein, F.; Luo, W.; Kirchlechner, C.; Dehm, G.: *Micromechanics of Laves Phases: Strength, Fracture Toughness, and Hardness as Function of Composition and Crystal Structure* (Joint EPRI-123 HIMAT Conference on Advances in High Temperature Materials. Nagasaki, Japan. 20 Oct. 2019)
- Stephenson, L.; Katnagallu, S.; Mouton, I.; Oliveira, F.; Gault, B.; Raabe, D.: *An Atomic Renaissance for Pulsed Field Ion Microscopy* (Microscopy & Microanalysis 2019. Portland, OR, USA. 04 Aug. 2019)
- Sun, B.; Krieger, W.; Ponge, D.; Rohwerder, M.; Raabe, D.: *Hydrogen embrittlement of medium Mn steels with ferrite matrix or austenite matrix* (4th High Manganese Steel 2019 HMnS. Aachen, Germany. 01 Apr. 2019)
- Surendralal, S.: *Implementation of an ab initio electrochemical potentiostat: Application to Mg corrosion* (Symposium "Fundamentals of the electrochemistry of the metal/electrolyte interface", Imperial College. London, UK. 25 Apr. 2019)
- Tehranchi, A.; Hickel, T.; Neugebauer, J.: *Atomistic simulations of hydrogen-defect interactions in metals* (Workshop "Hydrogen in Metals - current understanding and future needs", St Anne's College. Oxford, UK. 18 Apr. 2019)
- Todorova, M.; Yoo, S.-H.; Surendralal, S.; Neugebauer, J.: *Modelling electrochemical solid/liquid interfaces by first principles calculations* (19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, ICTP. Trieste, Italy. 10 Jan. 2019)
- Todorova, M.; Yoo, S.-H.; Surendralal, S.; Neugebauer, J.: *A fully ab initio approach to electrochemistry and corrosion* (CNLS Colloquium, Los Alamos National Laboratory. Los Alamos, NM, USA. 28 Jan. 2019)
- Todorova, M.; Surendralal, S.; Neugebauer, J.: *First-principles approach to model electrochemical reactions at the solid-liquid interface* (Spring Meeting of the German Physical Society (DPG). Regensburg, Germany. 03 Apr. 2019)
- Todorova, M.; Yoo, S.-H.; Surendralal, S.; Neugebauer, J.: *A fully ab initio approach to modelling electrochemical solid/liquid interfaces* (Chemiekolloquium der Johannes Kepler Universität Linz. Linz, Austria. 14 May 2019)
- Todorova, M.; Surendralal, S.; Neugebauer, J.: *Building an ab-initio potentiostat in a standard DFT code with periodic boundary conditions* (ELRC2019 - IPAM reunion workshop. Lake Arrowhead, CA, USA. 14 Jun. 2019)
- Todorova, M.; Yoo, S.-H.; Surendralal, S.; Neugebauer, J.: *Ab initio approach to electrochemistry and corrosion* (Computational Materials Chemistry Workshop. Telluride, CO, USA. 16 Jul. 2019)
- Todorova, M.; Surendralal, S.; Neugebauer, J.: *Degradation processes at surfaces and interfaces* (ISAM4: The fourth International Symposium on Atomistic and Multiscale Modeling of Mechanics and Multiphysics, Friedrich-Alexander Universität Erlangen-Nürnberg (FAU). Erlangen, Germany. 07 Aug. 2019)



Todorova, M.; Yoo, S.-H.; Surendralal, S.; Neugebauer, J.: *Predicting atomic structure and chemical reactions at solid-liquid interfaces by first principles* (Operando surface science – Atomistic insights into electrified solid/liquid interfaces (708. WE-Heraeus-Seminar), Physikzentrum. Bad Honnef, Germany. 10 Dec. 2019)

Zaefferer, S.: *Electron diffraction techniques in scanning electron microscopy: fundamentals and state-of-the-art applications of electron backscatter diffraction (EBSD) and electron channelling contrast imaging (ECCI)* (27th Annual Meeting of the German Crystallographic Society (DGK). Leipzig, Germany. 25 Mar. 2019)

Zaefferer, S.: *In-situ electron channeling contrast imaging (ECCI) to observe the effect of hydrogen in TWIP steels and superalloys* (Physikalisches Kolloquium der Universität Wien. Wien, Austria. 29 Jan. 2019)

Zaefferer, S.: *Investigation on the effect of hydrogen on dislocation patterns in high-strength steels using electron channelling contrast imaging in the scanning electron microscope* (15th Multinational Congress on Microscopy. Belgrade, Serbia. 15 Sep. 2019)

Zaefferer, S.: *Measurement of local residual stresses using cross-correlation EBSD and ring core milling* (27th International Conference on Materials and Technology (26 ICM&T). Portoroz, Slovenia. 16 Oct. 2019)

Zaefferer, S.: *Microstructure Characterization in 2D and 3D using Advanced SEM-based Electron Diffraction Techniques* (3rd Materials Genome Engineering Forum. Kunming, China. 23 Nov. 2019)

Zaefferer, S.: *Microstructure Characterization in 2D and 3D using Advanced SEM-based Electron Diffraction Techniques* (Chongqing University Colloquium. Chongqing, China. 26 Nov. 2019)

Zaefferer, S.: *Residual stress measurements on steel using cross-correlation EBSD and ring core milling* (EDAX workshop. Weiterstadt, Germany. 30 Oct. 2019)

Zaefferer, S.: *Understanding hydrogen-embrittlement during fatigue loading of a high-Mn-steel using ECCI and CC-EBSD* (RMS-EBSD conference. London, UK. 03 Apr. 2019)

Zaefferer, S.; An, D.: *Hydrogen-induced embrittlement during fatigue loading of a high-Mn steel investigated by electron channelling contrast imaging (ECCI)* (Euromat 2019. Stockholm, Sweden. 01 Sep. 2019)

Zaefferer, S.; Nandy, S.; Sandlöbes, S.; Raabe, D.: *Understanding the ductilization effect in Mg alloyed with Ca, Al, and Zn* (Euromat 2019. Stockholm, Sweden. 01 Sep. 2019)

Zaefferer, S.; Shan, Y.; Madivala, M.: *Nano-indentation and electron channelling contrast imaging (ECCI) to understand the interaction of hydrogen and dislocations in a high-Mn TWIP steel* (Euromat 2019. Stockholm, Sweden. 01 Sep. 2019)

Zhang, S.: *Electron Microscopy* (DGK-AK20 Summer School "Synthesis and characterization of inorganic

functional materials." Mülheim (Ruhr), Germany. 22 Jul. 2019)

Zhang, S.: *Modern electron microscopy goes high dimensions: handling big data* (BIG DATA SUMMER – BiGmax Network. Platja d'Aro, Spain. 09 Sep. 2019)

2020

Antonov, S.: *Overview of the Damage Accumulation Mechanisms During Non-isothermal Creep of Ni-based superalloys* (Seminar, Exponent, online. Atlanta, GA, USA. 18 Dec. 2020)

Antonov, S.; Tan, Q.; Gault, B.: *Atom Probe Tomographic Investigation of the Solute Segregation to Crystal Defects in γ -phase Co-35Ni-20Cr-10Mo Superalloy* (Microscopy & Microanalysis (M&M) Meeting, virtual. Milwaukee, WI, USA. 01 Aug. 2020)

Best, J. P.: *Connecting structure to the micro-mechanics and macro-scale fracture toughness of a laser-processed BMG using micro-focussed high-energy X-rays at PETRA III* (PETRA IV Workshop – Earth, Environment, and Materials for Nanoscience and Information Technology, online. Hamburg, Germany. 02 Nov. 2020)

Best, J. P.: *Nano-/Micromechanics of Materials: A focus on laser-processed BMGs* (Deutsches Zentrum für Luft- und Raumfahrt (DLR) Seminar Series, online. Köln, Germany. 01 Dec. 2020)

Best, J. P.: *Small-scale mechanics at the Max-Planck-Institute in Düsseldorf: An overview* (Oxford Materials Group Seminar Series, online. Oxford, UK. 27 Aug. 2020)

Dehm, G.: *Micro- and Nanomechanical Testing of Materials - From Methods to Mechanical Properties* (SFB 1394 Summer School, online. Aachen, Germany. 05 Oct. 2020)

Dehm, G.: *Resolving grain boundary phase transformations in Copper by advanced STEM* (TimeMan, online. Lille, France. 22 Oct. 2020)

Diehl, M.; Cereceda, D.; Marian, J.; Liu, C.; Dong, J.; Wicke, M.; Brückner-Foit, A.; Kamachali, R. D.; Shanthraj, P.; Roters, F.; Eisenlohr, P.; Raabe, D.: *Coupling Crystal Plasticity and Phase Field Methods - The Future of Integrated Computational Materials Engineering?* (Seminar "Materials Technology, in particular of Magnesium Materials." Geesthacht, Germany. 17 Jan. 2020)

Diehl, M.; Kusampudi, N.; Kusche, C.; Raabe, D.; Korte-Kerzel, S.: *Combining Experiments, Simulations, and Data Science to Understand Damage in Dual Phase Steels* (International Conference on Plasticity, Damage, and Fracture. Riviera May, Mexico. 03 Jan. 2020)

Duarte, M. J.; Fang, X.; Rao, J.; Dehm, G.: *Hydrogen-microstructure interactions at small scale by in-situ nanoindentation during hydrogen charging* (Nanobrücken 2020: A nanomechanical Testing Conference. Düsseldorf, Germany. 05 Feb. 2020)

Eisenlohr, P.; Chakraborty, A.; Shanthraj, P.; Diehl, M.; Pagan, D.; Bieler, T. R.: *More than Crystal Plasticity: Multi-*

physics in DAMASK (TMS 2020. San Diego, CA, USA. 23 Jan. 2020)

Gault, B.: *An introduction to atom probe tomography: from fundamentals to atomic-scale insights into engineering materials* (Rolls Royce Lunch Time Seminar. Derby, UK. 01 Jul. 2020)

Gault, B.: *Pushing the limits of atomic-scale analytical microscopy* (London Centre for Nanoscience Lunch Time Seminar, online. London, UK. 11 Nov. 2020)

Gault, B.; Kim, S.-H.; Lim, J.; El-Zoka, A.; Kasian, O.; Sahu, R.; Stephenson, L.; Scheu, C.: *Nanoparticle Specimen Preparation for Atom Probe: Chemical Fixation and... cryo-Fixation (?)* (TMS 2020. San Diego, CA, USA. 23 Feb. 2020)

Gault, B.; Kwiatkowski da Silva, A.; Zhao, H.; Ponge, D.; Raabe, D.: *Atom probe tomography for studying the interplay of segregation and phase transformations* (17th International Conference on Aluminium Alloys, online. Grenoble, France. 26 Oct. 2020)

Güder, Ü.: *Archaeo-metallurgical Studies on Objects and Slags from the Persian period Iron Smithy in Tel Akko* (Early Iron Production: Experimental Archaeology, The Southern Levant and Africa, Research Workshop of the Israel Science Foundation. Ariel, Israel. 02 Feb. 2020)

Herbig, M.: *Material alterations in intense mechanical and chemical contacts* (TMS 2020. San Diego, CA, USA. 23 Feb. 2020)

Hickel, T.; Aydin, U.; Sözen, H. I.; Dutta, B.; Pei, Z.; Neugebauer, J.: *Innovative concepts in materials design to boost renewable energies* (Seminar of Institute for Innovative Technologies, SRH Berlin University of Applied Sciences. Berlin, Germany. 15 Jan. 2020)

Hickel, T.; McEniry, E.; Nazarov, R.; Dey, P.: *Ab initio basierte Simulation zur Wasserstoffversprödung in hoch-Mn Stählen* (Seminar der Staatlichen Materialprüfungsanstalt Darmstadt, Institut für Werkstoffkunde. Darmstadt, Germany. 21 Jan. 2020)

Hickel, T.: *Application of Density Functional Theory in the Context of Phase Diagram Modelling* (MSIT Winter School on Materials Chemistry, Virtual Event. Castle Ringberg, Tegernsee. 16 Feb. 2020)

Hickel, T.; Janßen, J.; Sözen, H. I.; Körmann, F.; Neugebauer, J.: *High-throughput optimization of finite temperature phase stabilities: Concepts and application* (IMWF Stuttgart, Colloquium Materials, virtual. Stuttgart, Germany. 10 Dec. 2020)

Janßen, J.; Hickel, T.; Neugebauer, J.: *Automated ab-initio Determination of Materials Properties at finite Temperatures with pyiron* (NIST Workshop, virtual. Rockville, MD, USA. 06 Aug. 2020)

Janßen, J.; Hickel, T.; Neugebauer, J.: *pyiron – an integrated development environment for ab initio thermodynamics* (AMS Seminar, virtual. Bochum, Germany. 05 Oct. 2020)

Körmann, F.; Ikeda, Y.; Srinivasan, P.; Dutta, B.; Neugebauer, J.; Grabowski, B.; Kostuchenko, T.; Shapeev, A.: *Ab Initio Phase Stabilities of High Entropy and Chemically Complex Alloys* (TMS 2020. San Diego, CA, USA. 27 Feb. 2020)

Liebscher, C.: *Strain and temperature induced phase transformations in high entropy alloys explored by in situ S/TEM* (Institute of Micro- and Nanostructure Research Colloquium, Friedrich-Alexander University Erlangen-Nürnberg, online. Erlangen, Germany. 25 Jun. 2020)

Liebscher, C.; Lu, W.; Dehm, G.; Raabe, D.; Li, Z.: *Complex phase transformation pathways in high entropy alloys explored by in situ S/TEM* (Third International Conference on High Entropy Materials. Berlin, Germany. 26 Sep. 2020)

Liebscher, C.; Lu, W.; Li, Z.; Raabe, D.; Dehm, G.: *Atomic scale in situ observations of phase transformations in complex alloy systems* (Integrated in-situ solutions for TEM – DENSsolutions, TVIPS and QuantumDesign Workshop. Gauting, Germany. 12 Feb. 2020)

Liebscher, C.; Meiners, T.; Peter, N. J.; Frolov, T.; Dehm, G.: *Atomic resolution observations of grain boundary phase transformations* (Gaseous Electronics Symposium (GES3). Rogla, Slovenia. 05 Feb. 2020)

Lymperakis, L.: *Nanomaterials from first principles* (Department of Physics Colloquium, University of Crete, delivered online. Crete, Greece. 05 Nov. 2020)

Lymperakis, L.: *Properties and design of nanomaterials from first principles* (Department of Physics Colloquium, University of Crete, delivered online. Crete, Greece. 05 Nov. 2020)

Mendive-Tapia, E.: *Ab initio origin of the short period magnetism of MnGe from thermally fluctuating local moments* (Quantum Theory of Materials Seminar, virtual. Jülich, Germany. 08 Jul. 2020)

Neugebauer, J.; Janßen, J.; Huber, L.; Ikeda, Y.; Körmann, F.; Grabowski, B.; Hickel, T.; Shapeev, A.: *Materials Design in High Dimensional Chemical and Structural Configuration Spaces* (TMS 2020. San Diego, CA, USA. 27 Feb. 2020)

Neugebauer, J.; Lymperakis, L.; Janßen, J.; Huber, L.; Hickel, T.: *Modeling crystal growth and materials design in high dimensional chemical and structural configuration spaces* (German Conference on Crystal Growth DKT 2020. München/Garching, Germany. 12 Mar. 2020)

Palm, M.: *Phase Equilibria and Phase Diagrams* (4th MSIT Winter School on Materials Chemistry. Online. 17 Feb. 2020)

Palm, M.: *Eisenaluminide* (DGM-WEBinar „Einführung in metallische Hochtemperaturwerkstoffe. Online. 13 May 2020)

Ponge, D.; Kwiatkowski da Silva, A.; Makineni, S. K.; Katnagallu, S.; Zhou, X.; Mianroodi, J. R.; Stephenson, L.; Kontis, P.; Freysoldt, C.; Gault, B.; Neugebauer, J.: *Chemistry and Structure at Lattice Defects studied at the Atomic Scale* (4th Symposium Core Research Cluster Materials

Science & 3rd Symposium on International Joint Graduate Program in Materials Science, Tohoku University, online. Tohoku, Japan. 16 Nov. 2020)

Raabe, D.: *Interplay of Chemistry and Structure at Lattice Defects studied at the Atomic Scale* (The 4th Symposium for The Core Research Cluster for Materials Science and the 3rd Symposium on International Joint Graduate Program in Materials Science "Create New Value of Materials Science through Broad Collaboration", Tohoku University, online. Sendai, Japan. 16 Nov. 2020)

Raabe, D.: *Theory-guided design of materials, microstructures and processes* (Workshop on the Future of Materials Science, Institute of Nanotechnology, KIT, online. Karlsruhe, Germany. 08 Jul. 2020)

Raabe, D.; Diehl, M.; Shanthraj, P.; Sedighiani, K.; Roters, F.: *Multi-scale and multi-physics simulations of chemo-mechanical crystal plasticity problems for complex engineering materials using DAMASK* (Online Colloquium Lecture, Department of Materials Science and Engineering, KTH Royal Institute of Technology. Stockholm, Sweden. 05 Jun. 2020)

Raabe, D.; Kim, S.-H.; Zhang, X.; Schweinar, K.; Souza Filho, I. R.; Ma, Y.; Stephenson, L.; El-Zoka, A.; Mianroodi, J. R.; Rohwerder, M.; Liliensten, L.; Paolantonio, M.; Thouden Sukumar, P.; Schneider, J. M.; Ponge, D.; Gault, B.: *Basic Research Opportunity and Leverage Effects in Sustainable Metallurgy* (Workshop: New Frontiers in Materials Science and Engineering – Sustainable Metallurgical Processes with improved CO₂ efficiency, RWTH Aachen, online. Aachen, Germany. 15 Sep. 2020)

Raabe, D.; Li, Z.; Ikeda, Y.; Dutta, B.; Körmann, F.; Neugebauer, J.: *Thermodynamics and symmetry effects in high entropy alloys* (Third International Conference on High Entropy Materials. Berlin, Germany. 26 Sep. 2020)

Ramachandramoorthy, R.: *High strain rate micromechanics: Instrumentation and implementation* (DGM - Arbeitskreis Rasterkraftmikroskopie und nanomechanische Methoden, online. 08 Jul. 2020)

Rohwerder, M.: *Strategies for enhancing Corrosion Protection by Organic Coatings* (71st Annual Meeting of the International Society of Electrochemistry, virtual. 31 Aug. 2020)

Roters, F.; Diehl, M.; Eisenlohr, P.; Shanthraj, P.: *DAMASK: the Düsseldorf Advanced Material Simulation Kit for studying multi-field crystal plasticity phenomena* (Seminar, Yanshan University, online. Qinhuangdao, Hebei, China. 09 Dec. 2020)

Roters, F.; Diehl, M.; Sedighiani, K.: *(Re-) formulation of dislocation density based crystal plasticity models in view of insights from parameter determination* (Oberwolfach Workshop: Mechanics of Materials: Towards Predictive Methods for Kinetics in Plasticity, Fracture, and Damage. Oberwolfach, Germany. 10 Mar. 2020)

Sahu, R.: *Study of phase impurity, 2D and 3D defects in orthorhombic MoAlB MAB phase* (Advances in Correlative Microscopy Workshop, IIT Madras. Chennai, India. 31 Jan. 2020)

Scheu, C.: *Atomic-scale characterization of complex solid solution nanoparticles using TEM* (Workshop on High Entropy Alloy and Complex Solid Solution Nanoparticles for Electrocatalysis, RUB, online. Bochum, Germany. 06 Oct. 2020)

Sedighiani, K.; Traka, K.; Diehl, M.; Roters, F.; Bos, K.; Sietsma, J.; Raabe, D.: *A Coupled Crystal Plasticity – Cellular Automaton Method for 3D Modeling of Recrystallization: Part I: Crystal Plasticity* (International Conference on Plasticity, Damage, and Fracture. Riviera May, Mexico. 03 Jan. 2020)

Stein, F.: *Experimental Determination of Phase Diagrams* (Lecture, 4th MSIT Winter School on Materials Chemistry. Castle Ringberg, Tegernsee. 16 Feb. 2020)

Stein, F.; Distl, B.; Palm, M.; Hauschildt, J.; Rackel, M. W.; Pyczak, F.; Mayer, S.; Yang, Y.; Chen, H.-L.; Engström, A.: *Improvement of a CALPHAD Database for the Development of Next Generation TiAl Alloys by Targeted Key Experiments on High-temperature Phase Equilibria – The EU Project ADVANCE* (Hume-Rothery Symposium: Phase Equilibria and Kinetics for Materials Design and Engineering, TMS 2020. San Diego, CA, USA. 23 Feb. 2020)

Todorova, M.: *Panel discussion leader* (BMBF-DOE bilateral workshop *Artificial Photosynthesis*, Virtual Discussion. Berlin, Germany. 24 Jun. 2020)

Todorova, M.; Yoo, S.-H.; Surendralal, S.; Neugebauer, J.: *Insights into the stability and reactivity of solid/liquid interfaces from ab initio calculations* (71st Annual Meeting of the International Society of Electrochemistry "Electrochemistry towards Excellence", virtual. Belgrade, Serbia. 03 Sep. 2020)

Traka, K.; Sedighiani, K.; Bos, K.; Lopez, J. G.; Diehl, M.; Angenendt, K.; Kestens, L.; Raabe, D.; Sietsma, J.: *A Coupled Crystal Plasticity – Cellular Automaton Method for 3D Modeling of Recrystallization: Part II: Subgrain Growth for Recrystallization* (International Conference on Plasticity, Damage, and Fracture. Riviera May, Mexico. 03 Jan. 2020)

Vercik, M.; Güder, Ü.: *Korrodiert, fragmentiert, zerbrochen. Die Aussagekraft der Eisenfunde aus dem Apollon-Heiligtum von Didyma* (Universität Hamburg, Archäologie und Kulturgeschichte des Antiken Mittelmeerraumes. Hamburg, Germany. 02 Dec. 2020)

Yoo, S.-H.: *Investigations of materials surfaces based on density functional theory calculations* (Department of Chemistry Seminar, Kangwon University, virtual. Chuncheon, Republic of Korea. 19 Nov. 2020)

Zaefferer, S.: *Combination of 2D and 3D SEM-based diffraction techniques with various other techniques for understanding of microstructures* (Workshop on correlative microscopy. Chennai, India. 31 Jan. 2020)

Zaefferer, S.: *Electron Channelling Contrast Imaging (ECCI) – A Technique for Observation and Quantitative In-situ Characterization of Crystal Lattice Defects in Bulk Samples* (12th Asia-Pacific Microscopy Conference (APMC 2020). Hyderabad, India. 03 Feb. 2020)

Zaefferer, S.: *Investigations on microstructural reasons for Goss texture formation in GO electrical steels - a search for the needle in the haystack* (9th International Conference Magnetism and Metallurgy. Rome, Italy. 03 Nov. 2020)

Zaefferer, S.: *Microstructure Characterization in 2D and 3D using Advanced SEM-based Electron Diffraction Techniques* (IISC Colloquium. Bangalore, India. 07 Feb. 2020)

Zaefferer, S.: *Towards understanding hydrogen embrittlement: Tools for microscopic and nanoscopic detection of hydrogen and its mechanical effects in microstructures of steels and superalloys* (International e-Conference on Structural Materials for Nuclear and Space Applications (SNSA20). Mumbai, India. 03 Dec. 2020)

Zhang, S.: *Efficiency and stability of catalytic nanostructures* (Colloquium, Ludwig-Maximilians-Universität. München, Germany. 13 Nov. 2020)

Zhao, H.; Gault, B.; De Geuser, F.; Huber, L.; Lu, W.; Peter, N. J.; Ponge, D.; Raabe, D.: *Segregation and precipitation at grain boundaries in an Al-Zn-Mg-Cu alloy* (17th International Conference on Aluminium Alloys ICAA 2020, virtual. Grenoble, France. 26 Oct. 2020)

Zhou, X.; Mianroodi, J. R.; Kwiatkowski da Silva, A.; Koenig, T.; Thompson, G. B.; Shanthraj, P.; Ponge, D.; Gault, B.; Svendsen, B.; Raabe, D.: *Revealing the dependence of Au segregation on dislocation character in Pt-Au via cross-correlative microscopy* (APT&M 2020, virtual. Oxford, UK. 16 Nov. 2020)

2021

Antonov, S.: *A primer to atom probe tomography and its application to intermetallics* (Intermetallics 2021. Bad Staffelstein, Germany. 04 Oct. 2021)

Antonov, S.: *Towards Improved Superalloy Performance via Defect Engineering* (Department of Mechanical Colloquium, Industrial, and Manufacturing Engineering, Oregon State University, online. Corvallis, OR, USA. 10 May 2021)

Antonov, S.: *Understanding phase transformations at boundaries and interfaces in β -Titanium alloys at the near-atomic scale* (Conference on Possibilities and Limitations of Quantitative Materials Modeling and Characterization. Bernkastel-Kues, Germany. 12 Oct. 2021)

Antonov, S.: *Understanding Superalloys on the Atomic Scale* (Department of Materials Science Colloquium, University of Illinois Urbana-Champaign, online. Urbana, IL, USA. 01 Mar. 2021)

Antonov, S.: *Understanding the Defect-Solute Interactions during Deformation of Superalloys* (Colloquium, Oak Ridge National Laboratory, online. Oak Ridge, TN, USA. 25 Jun. 2021)

Antonov, S.; Shi, R.; Li, D.; Kloenne, Z.; Zheng, Y.; Fraser, H. L.; Raabe, D.; Gault, B.: *Atom Probe Tomographic Study of Precursor Metastable Phases and Their Influence on a Precipitation in the Metastable β -titanium Alloy, Ti-5Al-*

5Mo-5V-3Cr (TMS 2021, online. Pittsburgh, PA, USA. 14 Mar. 2021)

Brink, T.: *From contact mechanics to wear* (EPFL Summer School: Tribology and Surfaces Interactions. Visp, VS, Switzerland. 23 Aug. 2021)

Dehm, G.: *Congruent and non-congruent grain boundary phase transformations in Copper studied by advanced STEM* (Virtual Seminar of Institute Jozef Stefan. Ljubljana, Slovenia. 04 Mar. 2021)

Dehm, G.: *Experimental Insights in Congruent and Non-Congruent Grain Boundary Phase Transformations in Copper by Advanced STEM* (International Seminars, Technion - Israel Institute of Technology (Israel), Purdue University (USA), virtual. 06 May 2021)

Dehm, G.: *Probing the local influence of micro- and nanostructure on mechanical properties of Materials* (E-MRS Spring Meeting, online. 31 May 2021)

G. Dehm: *Probing The Local Influence Of Materials' Nanostructure On Mechanical Properties* (Anhui University of Technology, School of Metallurgical Engineering, Ma'anshan, China, online. 04 Nov. 21)

G. Dehm, T. Meiners, J. Duarte, T. Frolov, C. Liebscher: *Atomic structure of two phases of a Cu tilt grain boundary resolved by scanning transmission electron microscopy* (MS&T, Columbus, USA, hybrid. 17 Oct. 21)

Dehm, G.; Peter, N. J.; Meiners, T.; Frommeyer, L.; Brink, T.; Frolov, T.; Liebscher, C.: *Grain boundary phases in pure and alloyed Cu: Insights from advanced STEM* (Microscopy Conference 2021 Joint Meeting of Dreiländertagung & Multinational Congress on Microscopy, Virtual Meeting. 22 Aug. 2021)

Diehl, M.; Kusampudi, N.: *Using machine learning and crystal plasticity simulation to design damage resistant dual phase steels* (Webinar: Metal Plasticity Seminar-Artificial Intelligence, Machine Learning and Big Data in Metal Plasticity. Leuven, Belgium. 01 Oct. 2021)

Duarte, M. J.: *Hydrogen effects on the mechanical behavior of Fe alloys at small scale* (Micromechanical and Macroscopic Modelling (MMM) Special Seminar, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, online. Bochum, Germany. 13 Jul. 2021)

Duarte, M. J.: *Metales y aleaciones bajo impacto ambiental: corrosión, fragilización por hidrógeno y propiedades mecánicas* (Primer Simposio "Materiales aplicados" del Capítulo Estudiantil de la Sociedad Mexicana de Materiales, Unidad Profesional Interdisciplinaria de Ingeniería, Campus Guanajuato, UPIIG IPN, online. Guanajuato, Mexico. 25 May 2021)

Duarte, M.J.; Rao, J.; Dehm, G.: *Hydrogen and micromechanics in ferritic alloys* (Oxford Materials Colloquium, online seminar. Oxford, United Kingdom. 4 Feb. 2021)

El-Zoka, A.: *Materials Degradation: Turning a problem into a solution* (Colloquium on Integrated Metallic Nanomaterials Systems. Hamburg, Germany. 30 Jun. 2021)



- El-Zoka, A.: *Towards Enhanced Atom Probe Tomography Characterization of Wet Corrosion Systems* (SCI Electrochemistry Postgraduate Conference. Manchester, UK. 11 Jun. 2021)
- Freysoldt, C.; Hickel, T.; Janßen, J.; Wang, N.; Zendegani, A.: *High-throughput optimization of finite temperature phase stabilities: Concepts and application* (Coffee with Max Planck, Virtual Seminar organized by the MPIE. Düsseldorf, Germany. 04 Feb. 2021)
- Gault, B.: *Advancing corrosion understanding with (cryo-) Atom Probe Tomography* (Imperial College London - Rolls Royce Corrosion Seminar, online. London, UK. 17 Jun. 2021)
- Gault, B.: *An overview of the state-of-the-art of hydrogen analysis by APT* (APT school 2021, online. Rouen, France. 26 Oct. 2021)
- Gault, B.: *Enabling Cryo-Atom Probe Tomography* (1st Grenoble Atom Probe Workshop, online. Grenoble, France. 16 Mar. 2021)
- Gault, B.: *Introduction to atom probe tomography: performance and opportunities in characterizing microstructures* (Metallic Microstructures: European Lectures Online. 20 May 2021)
- Gault, B.: *Machine-Learning for Atom Probe Tomography* (Workshop "Research-data management, machine learning and material informatics for Superalloys", online. Bochum, Germany. 17 Jun. 2021)
- Gault, B.: *Pushing the analytical limits of atom probe tomography via cryo-enabled workflows* (Microscience Microscopy Congress 2021, online. Oxford, UK. 08 Jul. 2021)
- Gault, B.: *Pushing the limits of atomic-scale analytical microscopy* (University of Bristol Seminar, online. Bristol, UK. 01 Mar. 2021)
- Gault, B.: *Theory and Advances in Atom Probe Tomography* (Canadian Centre for Electron Microscopy Summer School, online. Hamilton, ON, Canada. 08 Jun. 2021)
- Gault, B.; Guillon, O.: *Du térawatt au picomètre: Voyage au cœur des technologies de l'hydrogène* (Café des Sciences de l'Ambassade de France en Allemagne, online. Berlin, Germany. 20 Jun. 2021)
- Güder, Ü.: *Archaeological Traces of High Carbon Steel Metallurgy in Anatolia* (The Iranian Highlands: Resiliences and Integration in Premodern Societies, Deutsches Bergbau-Museum Bochum, online. Bochum, Germany. 20 Oct. 2021)
- Güder, Ü.: *Following the fingerprints of ancient blacksmiths: reverse engineering of archaeological iron* (Pint of Science, online. Düsseldorf, Germany. 17 May 2021)
- Güder, Ü.: *Historical and Technological Assessment of New Metals in Anatolia: Zinc in Urartian Bronze Alloys* (Seminar, Institute of Archaeology, Charles University, online. Prague, Czech Republic. 10 Nov. 2021)
- Hickel, T.; Freysoldt, C.; Janßen, J.; Wang, N.; Zendegani, A.: *High-throughput optimization of finite temperature phase stabilities: Concepts and application* (Coffee with Max Planck, Virtual Seminar organized by the MPIE. Düsseldorf, Germany. 04 Feb. 2021)
- Hickel, T.: *Application of Density Functional Theory in the Context of Phase Diagram Modelling* (MSIT Winter School on Materials Chemistry, Virtual Event. 02 May 2021)
- Hickel, T.; Janßen, J.; Sözen, H. I.; Körmann, F.; Surendralal, S.; Todorova, M.; Neugebauer, J.: *High-throughput optimization of finite temperature phase stabilities: Concepts and application* (Thermec 2021, Virtual Conference. Graz, Austria. 11 May 2021)
- Hickel, T.; Janßen, J.; Sözen, H. I.; Srrekala, L.; Körmann, F.; Surendralal, S.; Todorova, M.; Neugebauer, J.: *High-throughput optimization of finite temperature phase stabilities: Concepts and application* (ICAMS Advanced Discussions, virtual. Bochum, Germany. 08 Jun. 2021)
- Huber, L.; Dsouza, R.; Poul, M.; Neugebauer, J.: *Defect Free Energies* (Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) Seminar, delivered online. Bochum, Germany. 19 Jan. 2021)
- Huber, L.: *Simulating the thermodynamics of GB phases* (Seminar, Institut für Materialwissenschaft (MaWi), University of Stuttgart, delivered online. Stuttgart, Germany. 08 Feb. 2021)
- Janßen, J.; Hickel, T.; Neugebauer, J.: *pyiron – an integrated development environment for ab initio thermodynamics* (Potential Workshop, ICAMS, virtual. Bochum, Germany. 13 Mar. 2021)
- Janßen, J.; Neugebauer, J.: *pyiron – an integrated development environment for material science* (CECAM Workshop, virtual. Lausanne, Switzerland. 25 Mar. 2021)
- Khanchandani, H.; Stephenson, L.; Raabe, D.; Zaefferer, S.; Gault, B.: *Investigation of hydrogen embrittlement in high Mn TWIP steel via correlative microscopy (ECCI, APT)* (Cameca Online Webinar series for Atom Probe Tomography. Jul. 2021)
- Kontis, P.; Antonov, S.; Kürnsteiner, P.; Katnagallu, S.; Mianroodi, J. R.; Liliensten, L.: *Development of superalloys driven by atomic-scale interactions of solutes with crystal defects* (TMS 2021, online. Pittsburgh, PA, USA. 15 Mar. 2021)
- Liebscher, C.: *How do grain boundaries transform in metallic alloys?* (Institute of Material Physics, Westfälische Wilhelms-Universität Münster, Online Colloquium. Münster, Germany. 15 Jun. 2021)
- Luo, T.; Gomell, L.: *Application of atom probe tomography in thermoelectrics research* (Cameca Online Webinar series for Atom Probe Tomography. Jun. 2021)
- Lymperakis, L.: *Nanomaterials from first principles* (Seminar: Programme of Postgraduate course Materials Physics and Technology, Department of Physics, Aristotle University of Thessaloniki. Thessaloniki, Greece. 14 May 2021)

Meiners, T.; Frolov, T.; Duarte, M. J.; Richter, G.; Liebscher, C.; Dehm, G.: *Resolving grain boundary phase transformations in Copper by advanced STEM* (Thermec 2021, Online Conference. 01 Jun. 2021)

Neugebauer, J.: *Ab initio guided design of compositionally complex alloys* (Materials for energy, Digital Workshop. Bochum, Germany. 26 Feb. 2021)

Neugebauer, J.; Surendralal, S.; Deißbeck, F.; Wippermann, S. M.; Freysoldt, C.; Todorova, M.: *Design and application of an ab initio electrochemical cell* (Spring Meeting of the German Physical Society (DPG), online. Berlin, Germany. 02 Mar. 2021)

Neugebauer, J.; Ikeda, Y.; Körmann, F.: *Materials design based on efficient sampling of high dimensional chemical and thermodynamic configuration spaces* (Workflows for Atomistic Simulations, Ruhr-Universität Bochum, Online Meeting. Bochum, Germany. 10 Mar. 2021)

Neugebauer, J.; Janßen, J.: *Pyiron – an integrated development environment for simulation workflows* (CECAM Summer School in 2020: "Simulation Workflows in Materials Modelling (SWiMM 2020)", CECAM HQ – École Polytechnique Fédérale de Lausanne, Virtual Meeting. Lausanne, Switzerland. 23 Mar. 2021)

Neugebauer, J.: *Materials design by exploiting high-dimensional chemical and structural configuration spaces* (Kolloquium im Rahmen des SFB 986, Technische Universität Hamburg-Harburg, Online Meeting. Hamburg-Harburg, Germany. 26 May 2021)

Neugebauer, J.; Zendegani, A.; Hickel, T.: *Defect phase diagrams as novel tool to understand and design tailored defect structures in advanced steels* (Thermec 2021, Virtual Meeting. Vienna, Austria. 03 Jun. 2021)

Neugebauer, J.: *First principles first* (ICAMS Advanced Discussions 2021: Recent trends in materials design, Virtual Conference. Bochum, Germany. 08 Jun. 2021)

Neugebauer, J.: *Panel discussion leader* (ICAMS Advanced Discussions 2021: Recent trends in materials design, Virtual Conference. Bochum, Germany. 08 Jun. 2021)

Neugebauer, J.: *Efficient sampling of high-dimensional chemical and thermodynamic configuration spaces* (ELRC2020: Invitation to Complex High-Dimensional Energy Landscapes Reunion Conference II, delivered online. Lake Arrowhead, CA, USA. 10 Jun. 2021)

Neugebauer, J.: *Ab initio descriptors to guide materials design in high-dimensional chemical and structural configuration spaces* (Münchener Physik Kolloquium - Festkolloquium für Professor Winfried Petry, Technische Universität München, delivered online. München, Germany. 21 Jun. 2021)

Neugebauer, J.; Surendralal, S.; Deißbeck, F.; Wippermann, S. M.; Todorova, M.: *Identifying and understanding corrosion reactions: An ab initio approach* (ICASS - 4th International Conference on Applied Surface Science, Virtual Conference. 30 Jun. 2021)

Neugebauer, J.: *Ab initio descriptors to guide materials design in high-dimensional chemical and structural configuration spaces* (EPFL Materials Science and Engineering (IMX) Seminar Series, virtual. Lausanne, Switzerland. 22 Nov. 2021)

Neugebauer, J.; Yoo, S.-H.; Lymperakis, L.: *Ab initio insights into fundamental intrinsic growth and materials limitations in group-III-nitrides* (MRS Fall Meeting, Virtual Conference, virtual. Boston, MA, USA. 28 Nov. 2021)

Palm, M.: *Phase Equilibria and Phase Diagrams* (5th MSIT Winter School on Materials Chemistry. Online. 3 May 2021)

Palm, M.: *Iron aluminides – a class of sustainable materials* (Intermetallics 2021, Educational Center Kloster Banz, Germany. 7 Oct. 2021)

Peter, N. J.: *Chemically triggered faceting transition of an asymmetric tilt grain boundary in Cu* (Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology, virtual. Bombay, India. 28 Jul. 2021)

Raabe, D.: *The Science of dirty alloys: recycling-based Aluminium for a circular economy* (The 4th International Conference on Light Materials - Science and Technology, online. 02 Nov. 2021)

Raabe, D.; Kim, S.-H.; Zhang, X.; Ma, Y.; Souza Filho, I. R.; Schweinar, K.; Angenendt, K.; Vogel, D.; Stephenson, L.; El-Zoka, A.; Mianroodi, J. R.; Rohwerder, M.; Gault, B.; Bai, Y.; Springer, H.; Ponge, D.; Kulse, M.; Mahajan, A.; Zaefferer, S.: *Sustainable Metals* (Virtual Keynote Perspective Lecture, Materials Chain and Materials Science Department, RUB. Bochum, Germany. 07 May 2021)

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Makineni, S. K.; Katnagallu, S.; Zhou, X.; Kamachali, R. D.; Stephenson, L.; Kontis, P.; Mianroodi, J. R.; Gault, B.; Thompson, G. B.; Neugebauer, J.: *Structure, chemistry and thermodynamics of Lattice Defects* (Colloquium of the Department of Materials Science and Engineering, Ohio State University, online. Columbus, OH, USA. 26 Mar. 2021)

Ramachandramoorthy, R.: *High strain rate testing from micro-to-meso scale* (MRS Spring Meeting - In Situ Mechanical Testing of Materials at Small Length Scales, Modeling and Data Analysis Symposium, online. 17 Apr. 2021)

Ramachandramoorthy, R.: *High strain rate testing of copper based micropillars and microlattices* (206 Departmental Seminar Series, Empa. Thun, Switzerland. 22 Jun. 2021)

Ramachandramoorthy, R.: *Micro/nanoscale fabrication techniques* (Small scale mechanics course, RUB. Bochum, Germany. 17 May 2021)

Ramachandramoorthy, R.: *Pushing the limits of microscale manufacturing and mechanical testing* (Department of Material Science and Engineering Seminar Series, Tel-Aviv University, online. Tel-Aviv, Israel. 18 May 2021)

Ramachandramoorthy, R.: *Small scale mechanical characterization* (Small scale mechanics course, RUB. Bochum, Germany. 31 May 2021)

Rohwerder, M.: *Scanning Kelvin Probe Techniques for the Investigation of Corrosion, Hydrogen Uptake and Permeation of Zinc Alloy Coatings on Steels* (Galvatech 2021, Virtual Conference. 21 Jun. 2021)

Roters, F.; Diehl, M.; Eisenlohr, P.; Shanthraj, P.: DAMASK: the Düsseldorf Advanced MATERIAL Simulation Kit for studying multi-field crystal plasticity phenomena (Seminar, Engineering Science Department at the University of Oxford, virtual. Oxford, UK. 18 Oct. 2021)

Scheu, C.; Gleich, S.; Soler, R.; Breitbach, B.; Bolvardi, H.; Achenbach, J.-O.; Schneider, J. M.; Dehm, G.: *Insights in the Structure, Defects and Stability of Mo₂BC Thin Films by Advanced Characterization Methods* (International Conference on Metallurgical Coatings and Thin Films 2021 (ICMCTF2021), Virtual Conference. 26 Apr. 2021)

C. Scheu: *Tracing impurities at surfaces and interfaces of renewable energy materials* (MS&T 21, Online Conference, Columbus, Ohio. 17 Oct. 2021)

Scheu, C.; Hengge, K. A.: *Insights in the stability of Pt/Ru catalyst and the effect for polymer electrolyte membrane fuel cells* (Thermec 2021, Online Conference. 01 Jun. 2021)

Scheu, C.; Zhang, S.: *Hematite for light induced water splitting – improving efficiency by tuning distribution of Sn dopants at the atomic scale* (Karlsruher Werkstoffkolloquium_Digital. 15 Jun. 2021)

Siemer, N.: *Metadata-schemes and RDM handbook in SFB1394* (Workshop “Research-data management, machine learning and material informatics within the SFB/TR103”, RUB, virtual. Bochum, Germany. 10 Jun. 2021)

Stein, F.: *Experimental Determination of Phase Diagrams* (Lecture, 5th MSIT Winter School on Materials Chemistry, virtual. 02 May 2021)

Surendralal, S.; Todorova, M.: *Corrosion at the Quantum Level* (Coffee with Max Planck, Virtual Seminar organized by the MPIE. Düsseldorf, Germany. 04 Feb. 2021)

Todorova, M.; Surendralal, S.: *Corrosion at the Quantum Level* (Coffee with Max Planck, Virtual Seminar organized by the MPIE. Düsseldorf, Germany. 04 Feb. 2021)

Todorova, M.; Surendralal, S.; Wippermann, S. M.; Deißbeck, F.; Freysoldt, C.; Neugebauer, J.: *Insights into processes at electrochemical solid/liquid interfaces from ab initio molecular dynamics simulations* (TMS 2021, online. Orlando, FL, USA. 16 Mar. 2021)

Todorova, M.; Surendralal, S.; Wippermann, S. M.; Deißbeck, F.; Neugebauer, J.: *Hydrogen at electrified solid/liquid interfaces – insights from ab initio molecular dynamics simulations* (TYC mini-workshop on “Physics and Chemistry of Solid/Liquid Interfaces”, online. London, UK. 20 May 2021)

Todorova, M.; Surendralal, S.; Wippermann, S. M.; Deißbeck, F.; Neugebauer, J.: *Insights into processes at electrochemical solid/liquid interfaces from ab initio molecular dynamics simulations* (ICTP-Workshop on “Physics and Chemistry of Solid/Liquid Interfaces for Energy Conversion and Storage”, Virtual Meeting. Trieste, Italy. 28 May 2021)

Todorova, M.; Yoo, S.-H.; Vatti, A. K.; Neugebauer, J.: *From Semiconductor defect chemistry to electrochemistry* (ICACES/BENCH Virtual Summer School 2021. Göttingen, Germany. 14 Jun. 2021)

Todorova, M.; Surendralal, S.; Wippermann, S. M.; Deißbeck, F.; Neugebauer, J.: *Insights into processes at electrochemical solid/liquid interfaces from ab initio molecular dynamics simulations* (ICACES/BENCH Virtual Summer School 2021. Göttingen, Germany. 14 Jun. 2021)

Todorova, M.; Surendralal, S.; Wippermann, S. M.; Deißbeck, F.; Neugebauer, J.: *Processes at solid/liquid interfaces – insights from ab initio molecular dynamics simulations with potential control* (AMaSiS 2021 Online - Applied Mathematics and Simulation for Semiconductors and Electrochemical Systems. Berlin, Germany. 06 Sep. 2021)

Todorova, M.; Surendralal, S.; Wippermann, S. M.; Deißbeck, F.; Neugebauer, J.: *Realistic description of processes at solid/liquid interfaces by ab initio molecular dynamics simulations with potential control* (MRS Fall Meeting. Boston, MA, USA. 7 Dec. 2021)

Tsai, S.-P.; Zaefferer, S.: *Large-volume 3D EBSD system and its application to the investigation of grain boundary corrosion in 316L stainless steel* (3D MS conference, online. 30 Jun. 2021)

Yoo, S.-H.: *Electronic passivation schemes for surfaces with spontaneous polarization and for low symmetry semiconductor surfaces in DFT slab calculations* (Materials Design Group Seminar, Department of Materials, Imperial College London, virtual. London, UK. 26 Apr. 2021)

Yoo, S.-H.: *Overcoming failing Size Convergence for Surface Calculations of Materials Exhibiting Spontaneous Polarization* (International Conference Materials Science and Engineering: Materials Oceania 2021, virtual. Brisbane City, Australia. 13 Oct. 2021)

Zaefferer, S.: *2D and 3D SEM-based electron diffraction techniques as central tools for correlative microscopy to obtain new insights into microstructure physics and chemistry* (Kolloquium des Zentrums für Elektronenmikroskopie, online. Graz, Österreich. 09 Mar. 2021)

Zaefferer, S.: *Towards understanding hydrogen embrittlement: Tools for microscopic and nanoscopic detection of hydrogen and its mechanical effects in microstructures of steels and superalloys* (Colloquium of the Institute of Materials Science, TU Freiberg, online. Freiberg, Germany. 10 May 2021)

Publications (as of November 2021)

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

Computational Materials Design:
<https://www.mpie.de/2967008/publications>

Interface Chemistry and Surface Engineering:
https://www.mpie.de/2999511/Interface_Chemistry_and_Surface_Engineering

Microstructure Physics and Alloy Design:
<https://www.mpie.de/2987664/Publications>

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

Nanoanalytics and Interfaces:
https://www.mpie.de/3118894/Nanoanalytics_and_Interfaces

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

Publication statistics

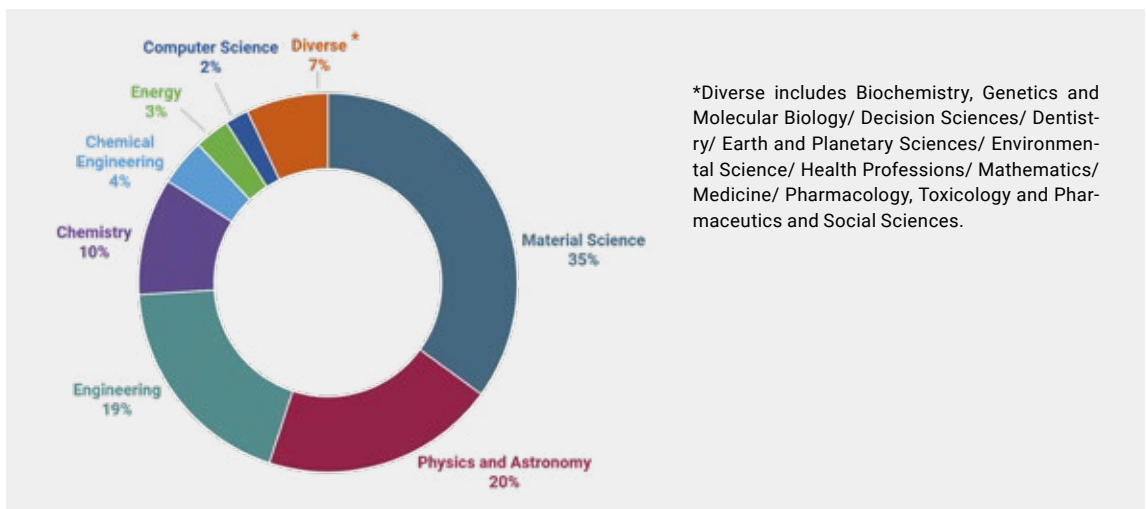
The results of the fundamental scientific research conducted at the MPIE are mainly published in peer-reviewed scientific journals. The following publication statistics are extracted from SciVal, which is based on the Scopus database of indexed scientific journals.^[1]

From January 2019 to November 2021, **831** peer-reviewed journal articles and reviews were published by the institute; over **50%** of the total set are **Open Access** and hence made broadly accessible across the scientific community but also the general public, with a mix between Gold and Green as detailed below.

Publications by subject area

High level subject areas for journals have been defined by the All Science Journal Classification (ASJC), and each journal and article therein can hence belong to more than one ASJC.^[1]

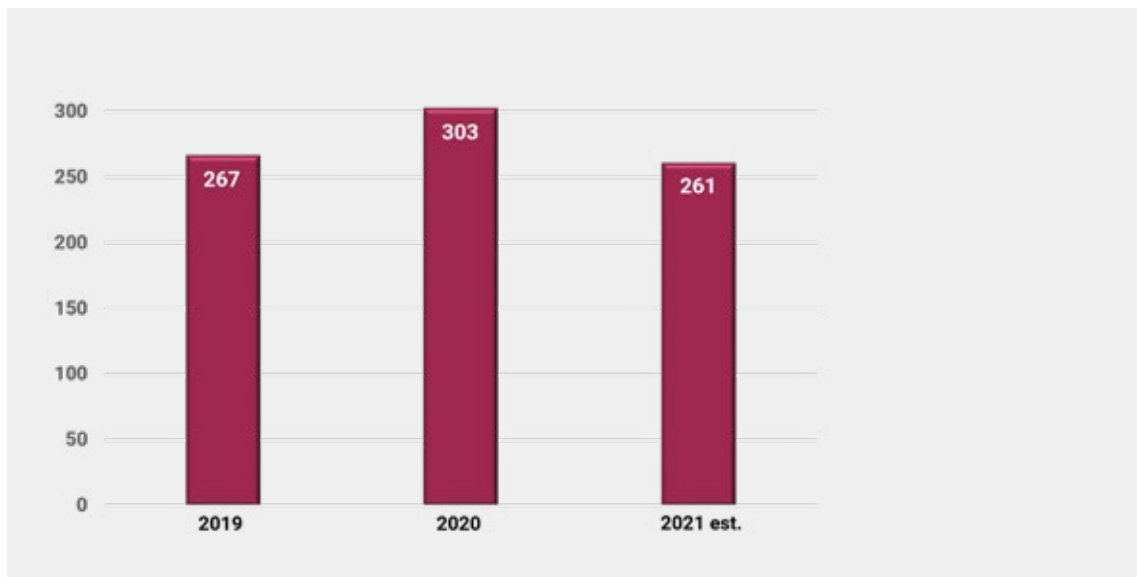
The set of publications between 2019 - 2021 from the MPIE cover a broad range of topics, centred on materials science & engineering and physics, but also with forays into chemistry, energy and computer science.





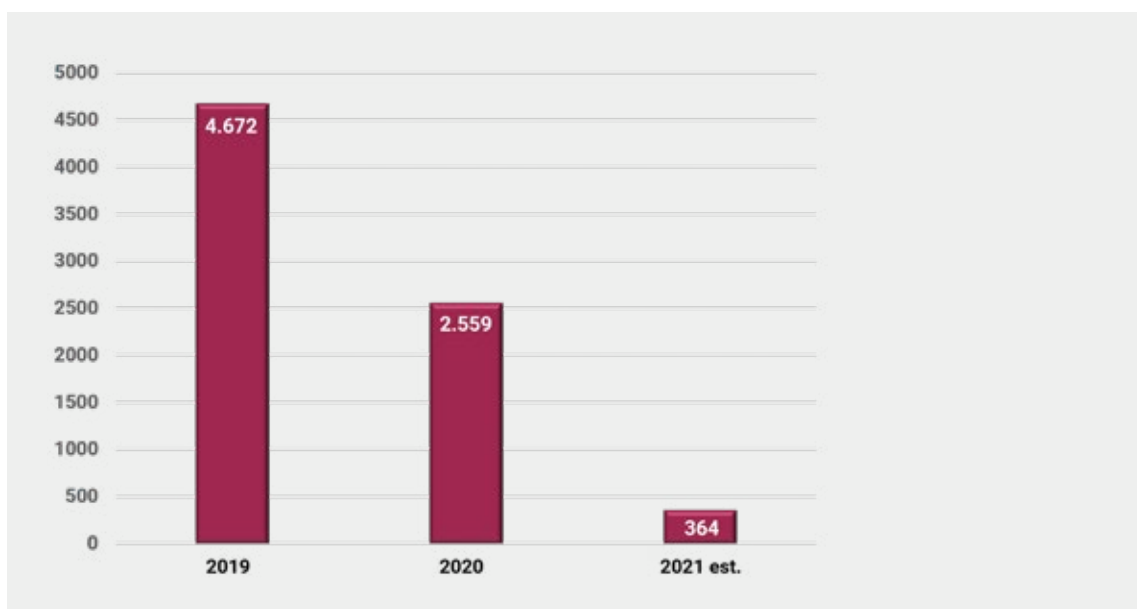
Scholarly output

A total of **831** publications was released until 24 November 2021.



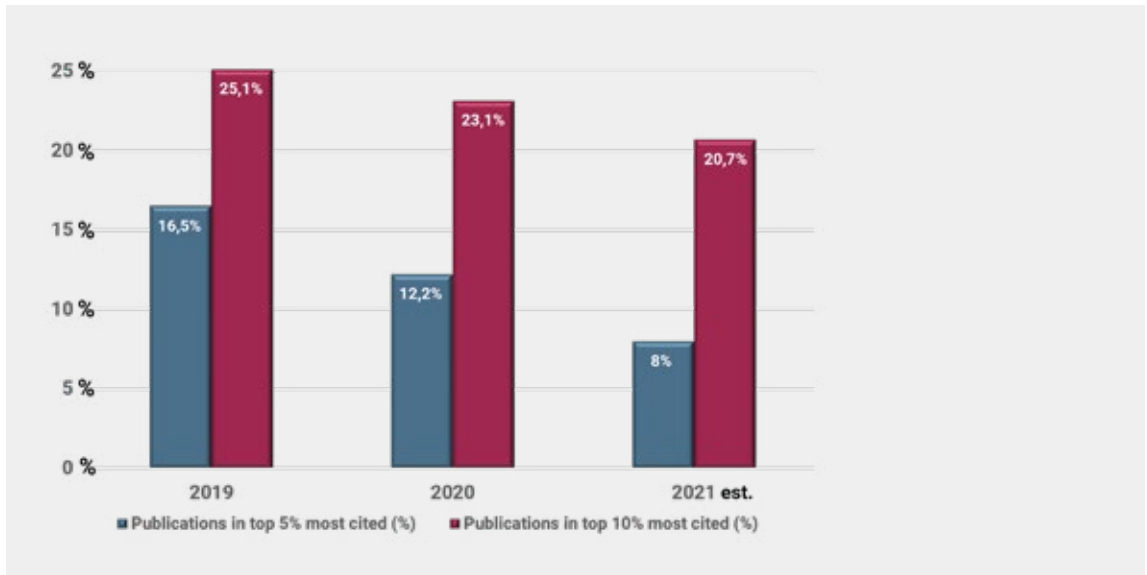
Citation count

A total of **7.595** citations was received by publications at the MPIE between 2019 – 2021 with **an average of 9.3** citations per publication. The citation count indicates how many citations these publications received. The years are always the years in which items were published, and do not refer to the years in which citations were received.



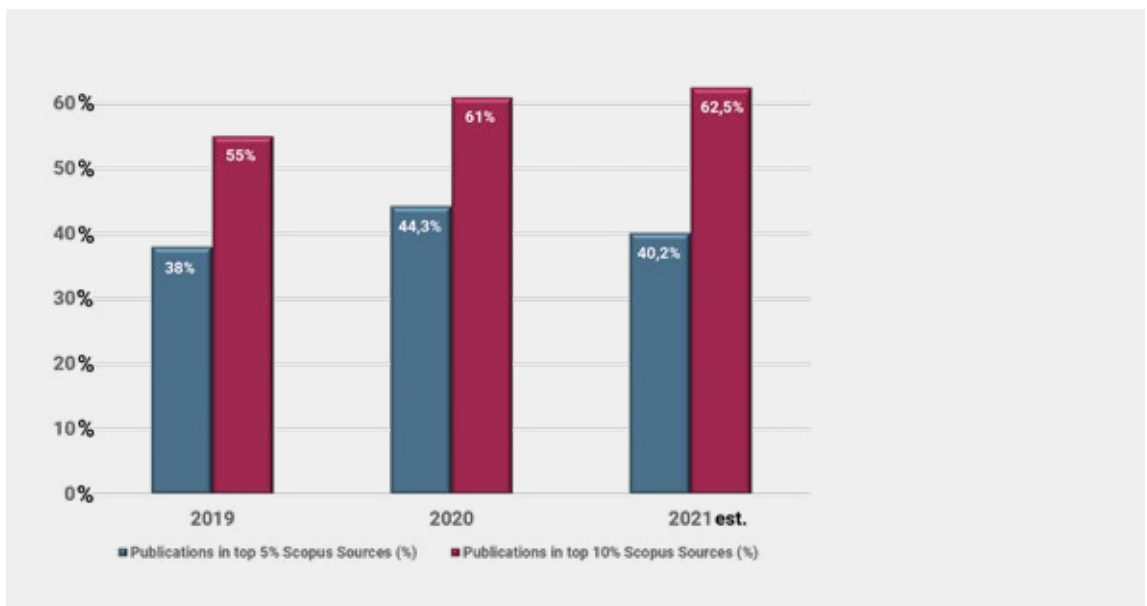
This is the total citations for the publication set, with years being the years when articles were published, not to the years in which citations were received. ^[1]

189 (23%) publications are **in the top 10% most cited publications** worldwide in their respective field.



482 (59,6%) publications are **in the top 10% journals** by CiteScore.

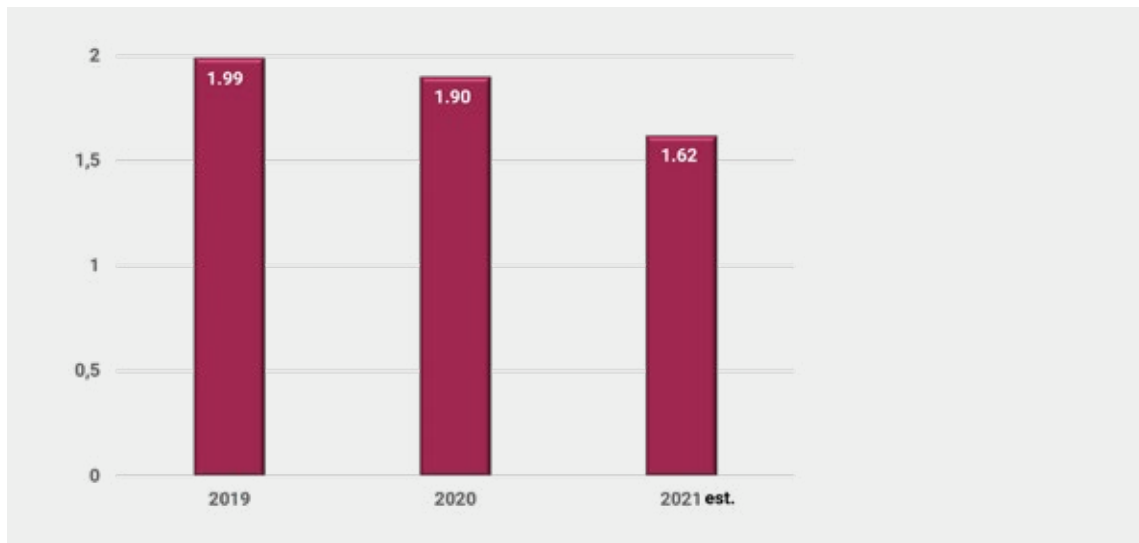
These values indicate the extent to which the set of publication from the MPIE is present in the most-cited journal articles referenced in Scopus, and presented by CiteScore percentile.^[1]



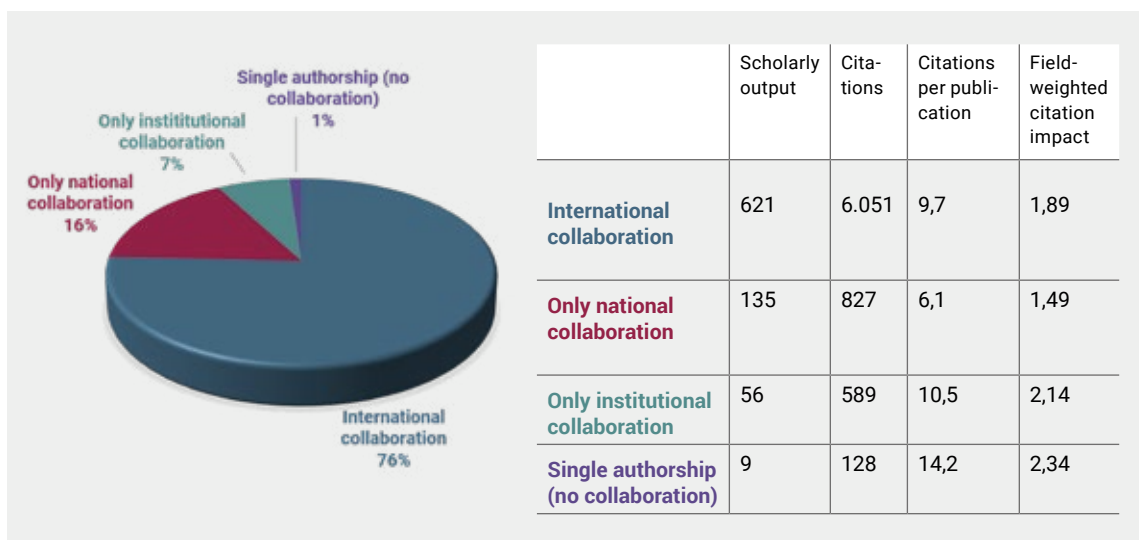


The field-weighted citation **impact** of publications at the MPIE is **1.85**.

The field-weighted citation impact (FWCI) indicates how the number of citations received by the considered set of publications compares with the average number of citations received by all other publications indexed in Scopus in similar categories. A FWCI of 1.00 indicates that the set has been cited exactly as would be expected based on the global average for similar publications across the considered field. A FWCI of more than 1.00 indicates above average citations.^[1]



Scholarly output in publications by amount of international, national and institutional collaboration



“The scholarly output in publications by amount of international, national and institutional collaboration indicates the extent to which the publication set’s publications have international, national, or institutional co-authorship, and single authorship. A publication is assigned a single collaboration type.”^[1]



Institutions participating in MPIE publications

Name	Scholarly output	Authors	Citations per publication
1. MPIE	821	344	9,3
2. Imperial College London	121	16	7,8
3. RWTH Aachen University	109	95	7,9
4. Central South University	62	46	10,0
5. Ruhr University Bochum	50	64	10,8
6. CNRS	47	80	6,5
7. Delft University of Technology	46	31	15,0
8. Jülich Research Centre	37	26	10,1
9. University of Science and Technology Beijing	36	69	7,2
10. Friedrich-Alexander University Erlangen- Nürnberg	31	24	13,1

Selected journals

Name	Number of publications
Acta Materialia	111
Scripta Materialia	56
Materials Science And Engineering A	40
Nature Communications	23
Physical Review B	14
Physical Review Letters	8
Advanced Materials	7
Science Advances	6
Nature	4
Nature Materials	4

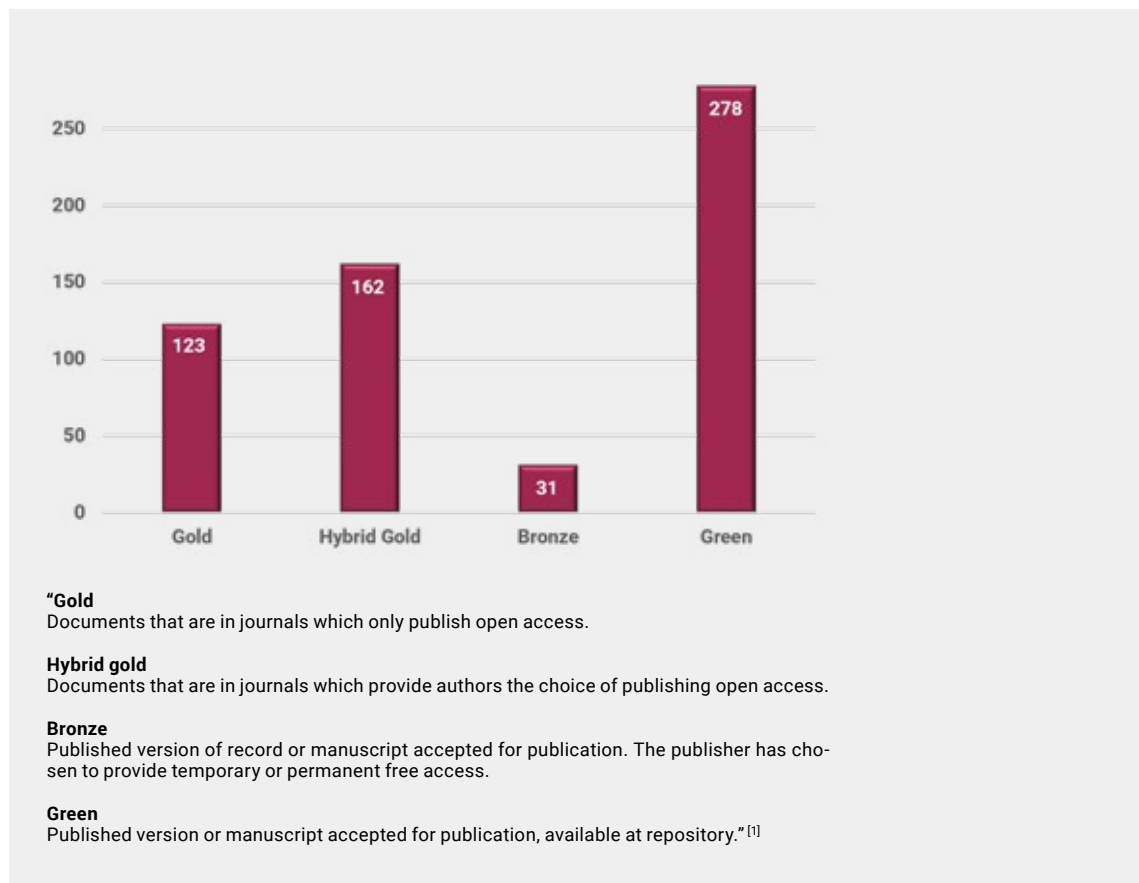


Open access

A total of **419** papers was published open access between 2019 and 2021.

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

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



References

1. SciVal, Publication Set Overview Report prepared on the 4th of November 2021.

Habilitation, doctoral, master and bachelor theses

Habilitation theses

2019

PD Dr. S. Brinckmann: Exploration of Crack Propagation in Metals by Length-Scale Dependent Simulations (Ruhr-Universität Bochum)

2021

PD Dr. M. Herbig: Hüftimplantate: Ein werkstoffwissenschaftlicher Blick auf Geschichte, Möglichkeiten und Limitationen (RWTH Aachen)

Doctoral theses

2018 (not included in Scientific Report 2016 - 2018)

Dr. rer. nat. M. Sysoltseva: Characterization of aerosols and nanoparticles released during various indoor and outdoor human activities (RWTH Aachen)

2019

Dr.-Ing. L. Abdellaoui: Correlation of microstructures and thermal conductivity of the thermoelectric material $\text{Ag}_{16.7}\text{Sb}_{30}\text{Te}_{53.3}$ (Ruhr-Universität Bochum)

Dr.-Ing. D. An: A study on low-cycle fatigue behaviour of high-manganese steels (RWTH Aachen)

Dr.-Ing. Y. Chang: Challenges and opportunities associated to the characterization of H/D in Ti and its alloys with atom probe tomography (RWTH Aachen)

Dr.-Ing. A. Dutta: Deformation behaviour and texture memory effect of multiphase nano-laminate medium manganese steels (RWTH Aachen)

Dr.-Ing. A. Gupta: Ab initio based study of precipitate formation in advanced structural Al-based alloys (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

Dr.-Ing. A. Hariharan: On the interfacial defect formation mechanism during laser additive manufacturing of polycrystalline superalloys (Ruhr-Universität Bochum)

Dr.-Ing. P. Kerger: Absolute Electrode Potentials - The Thin Film Electrode (Ruhr-Universität Bochum)

Dr.-Ing. A. Kini: Laser Additive Manufacturing of Oxide Dispersion Strengthened Steels and Cu-Cr-Nb Alloys (RWTH Aachen)

Dr.-Ing. D. Korbmacher: Ab initio study of strongly anharmonic and dynamically unstable systems (Ruhr-Universität Bochum)

Dr. rer. nat. P. Kürnsteiner: Precipitation Reactions During the Intrinsic Heat Treatment of Laser Additive Manufacturing (RWTH Aachen), **with distinction "summa cum laude"**

Dr.-Ing. W. Luo: Mechanical properties of the cubic and hexagonal NbCo_2 Laves phases studied by micromechanical testing (Ruhr-Universität Bochum)

Dr.-Ing. T. Meiners: Grain Boundary Structure, Phase Transitions and Segregation Phenomena in Copper Alloys (Ruhr-Universität Bochum)

Dr.-Ing. A. Merz: Investigation of the "Protection Zone", a novel mechanism to inhibit delamination of composite organic coatings containing conducting polymer (Ruhr-Universität Bochum)

Dr.-Ing. H.I. Sözen: Ab initio phase stabilities of Ce-based hard magnetic materials (Ruhr-Universität Bochum)

Dr. rer. nat. S. Tecklenburg: Defect formation and evolution in zinc oxide: from semiconductors to corrosion (Ruhr-Universität Bochum)

Dr.-Ing. M. Uebel: Release and transport of corrosion inhibitors in self-healing coatings for intelligent corrosion protection (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

Dr.-Ing. D. Wang: Damage and Strain Patterning Simulation of Structural Heterogeneity (RWTH Aachen)

Dr.-Ing. C.-H. Wu: The Principle and Applications of Scanning Kelvin Probe based Hydrogen Detection Technique on Pd-coated and Oxide Covered Surface (Ruhr-Universität Bochum)

Dr.-Ing. H. Zhao: Segregation and precipitation at interfaces in a model Al-Zn-Mg-Cu alloy (RWTH Aachen)

2020

Dr.-Ing. V.G. Arigela: Development and application of a high-temperature micromechanics stage with a novel temperature measurement approach (Ruhr-Universität Bochum)

Dr.-Ing. P. Bajaj: Precipitation during Intrinsic Heat Treatment in Laser Additive Manufacturing (RWTH Aachen)

Dr.-Ing. C. Corrêa da Silva: Investigation of the kinetics of selective oxidation of iron model alloys during simulated (Ruhr-Universität Bochum)



Dr.-Ing. P. Keuter: Design of materials with anomalous thermophysical properties and desorption-assisted phase formation of intermetallic thin films (RWTH Aachen University), **with distinction "summa cum laude"**

Dr.-Ing. J. Li: Probing dislocation nucleation in grains and at Σ3 twin boundaries of Cu alloys by nanoindentation (Ruhr-Universität Bochum)

Dr.-Ing. S. Nandy: Investigations on the Mechanisms of Ductilization of Mg Alloys with Ca, Al and Zn (Ruhr-Universität Bochum)

Dr.-Ing. R. Pei: Microstructural Relationships of Strength and Ductility in a Newly Developed Mg–Al–Zn Alloy for Po-tential Automotive Applications (RWTH Aachen)

Dr.-Ing. Y. Qin: Microstructure alterations in bearing steels exposed to severe plastic deformation (RWTH Aachen)

Dr. M. Schestakow: Nanostrukturierte Cellulose-Aerogel-Polyesterverbunde (RWTH Aachen University), **with distinction "summa cum laude"**

Dr.-Ing. S. Surendralal: Development of an ab initio computational potentiostat and its application to the study of Mg corrosion (Ruhr Universität Bochum), **with distinction "summa cum laude"**

Dr.-Ing. S.-H. Yoo: Development of a computational framework to determine the chemical and thermodynamic stability of electrode materials in an electrochemical environment (Ruhr-Universität Bochum)

Dr.-Ing. A. Zendegani: Ab initio based study of the thermodynamics of complex intermetallics (Ruhr-Universität Bochum)

2021

Dr. rer. Nat. J. Janßen: pyiron – an Integrated Development environment for ab initio Thermodynamics (Paderborn University), **with distinction "summa cum laude"**

Dr.-Ing. S.-H. Kim: Engineering Impurities in Colloidal Nanostructures used in "Green Hydrogen" Generation (RWTH Aachen University), **with distinction "summa cum laude"**

Dr. rer. Nat. F. Lochner: Interplay of Real Space and Electronic Structure for Iron-Based Superconductors: An ab initio Study (Ruhr-University-Bochum)

Dr. D. Mayweg: Microstructural characterization of white etching cracks (RWTH Aachen)

Dr.-Ing. S.A.H. Motaman: Modeling of the microstructural effects on the mechanical response of poly-crystals (RWTH Aachen)

Dr. M. Obermaier: Development of characterization methods to improve automotive PEMFC degradation analysis (RWTH Aachen)

Dr.-Ing. N.J. Peter: Structure, chemistry and nanomechanics of grain boundaries in Cu–Ag alloys (Ruhr-Universität Bochum)

Dr. Z. Rao: Design of Invar and Magnetic High-Entropy Alloys (RWTH Aachen)

Dr.-Ing. K. Schweinar: Advancements in the understanding of Ir-based water splitting catalysts at the near-atomic scale (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

Dr. mont. L. Stemper: Crossover-alloys – a new approach for future aluminum alloys (University Leoben, Austria), **with distinction "summa cum laude"**

Dr.-Ing. C. Tian: On the damage initiation in dual phase steels: Quantitative insights from in situ micromechanics (Ruhr-Universität Bochum)

Dr.-Ing. P.-Y. Tung: Fundamentals of carbide decomposition and stability (Ruhr-Universität Bochum)

Dr.-Ing. S. Vakili: Multi-Phase-Field Modeling of Structure Formation in Metallic Foams (Ruhr-Universität Bochum)

Dr.-Ing. R.S. Varanasi: Mechanisms of refinement and deformation of novel ultrafine-grained medium manganese steels with improved mechanical properties (Ruhr-Universität Bochum)

Dr. rer. nat. Y. Wei: Machine learning methods in data-driven nanostructure analysis of materials (RWTH Aachen)

Dr.-Ing. S. Wolff-Goodrich: Development of AlCrFeNiTi Compositionally Complex Alloys for High Temperature Structural Applications (Ruhr-Universität Bochum)

Master theses

2019

R. Aymerich Armengol: Structure-property relationship studies of Pt/TiO₂ nanomaterials for electrochemical applications (Universitat Autònoma de Barcelona, Spain)

R. Bueno Villoro: Effect of the processing route on the microstructure of Ag₁₈Sb₂₉Te₅₃ (AST) based thermoelectrics (Universitat Autònoma de Barcelona, Spain)

R. Dsouza: Fully anharmonic self-diffusion coefficients using the Finite-Temperature String method (Ruhr-Universität Bochum)

F. Farzam: Microstructure Evolution in FCC Metals during Friction (Heinrich-Heine-Universität Düsseldorf)

U. Gajera: Phase diagrams derived from optimized empirical potentials (Ruhr-Universität Bochum)

D.R. Machado: Investigation of the low cyclic fatigue behavior of high manganese steels (RWTH Aachen)

S. Roongta: A Physics Based Crystal Plasticity Model for Cyclic Deformation (Ruhr-Universität Bochum)

H.C. Sam: Role of microstructure and environment on delayed fracture in a novel lightweight medium manganese steel (Augsburg University)

2020

A. Aslam: Thermodynamics of binary alloys at atomistic scale (Ruhr-Universität Bochum)

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

N. Kusampudi: Using Machine Learning and Data-driven Approaches to Predict Damage Initiation in Dual-Phase Steels (Ruhr-Universität Bochum)

L. Lahn: On the role of defects in Ir-Ru alloys for energy conversion applications (RWTH Aachen)

A. Saxena: Machine learning the formation of defect phases in aluminium alloys (Ruhr-Universität Bochum)

C.K. Soundararajan: Recrystallization behavior and mechanical properties of interstitially alloyed CoCrFeMnNi equiatomic high entropy alloy (RWTH Aachen University)

2021

Ç. Aras: Anharmonic free-energy calculation of dynamically unstable crystal structures (RWTH Aachen)

V. Bhuva: Algorithms for optimal chemical ordering (University of Passau)

B. Hill: Scanning electron microscopy study of the microscale degradation mechanisms in polymer electrolyte fuel cells (Heinrich-Heine-Universität Düsseldorf)

A. Kokot: Solidification and precipitated structure of $\text{Al}_{20}\text{Co}_x\text{Cr}_{20}\text{Fe}_{35}\text{Ni}_{20-x}\text{Ti}_5$ ($x = 0, 10, 20$) compositionally complex alloys (Heinrich-Heine-Universität Düsseldorf)

P. Mathews: Concentration-dependent finite temperature effects in metallic alloys (Ruhr-Universität Bochum)

A.W. Paiva do Nascimento: An optimized method to determine initial parameters of advanced yield surfaces for sheet metal forming applications (Ruhr-Universität Bochum)

M. Vega Paredes: Electron microscopy degradation studies of ruthenium-platinum core-shell nanoparticles for polymer electrolyte membrane fuel cells (Universitat Autònoma de Barcelona, Spain)

Bachelor theses

2020

M. Vega Paredes: Degradation mechanisms during operation of high temperature polymer electrolyte membrane fuel cells (Universitat Autònoma de Barcelona, Spain)

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 2007)

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

Prof. Jörg Neugebauer

Member (since 2004) and speaker (since 2014) 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 IT-advisory board (BAR) of the Max-Planck-Society (since 2006)

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

Member of the Scientific Committee of the PSI-k charity and Speaker of the Working Group Applications to real materials: Structural materials (since 2009)

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

Elected chair of the Metals and Materials (MM) Division of the German Physical Society (DPG) (2016 - 2019)

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

Elected member of the DFG review board (DFG-Fachkollegium) „Materials Science“ (2016 - 2020)

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

Foreign Member of the Austrian Academy of Sciences (since 2012)

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

Associate Editor, npj Computational Materials (since 2015)

Member of the scientific advisory board of the Physics Department of the University of Jena (2015 - 2020)

Member of the scientific advisory board GraFOx, Graduate school of several Leibniz institutes in Berlin

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)

Member of the High Entropy Alloys (HEA 2021) Conference International Advisory Committee (since 2021)

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

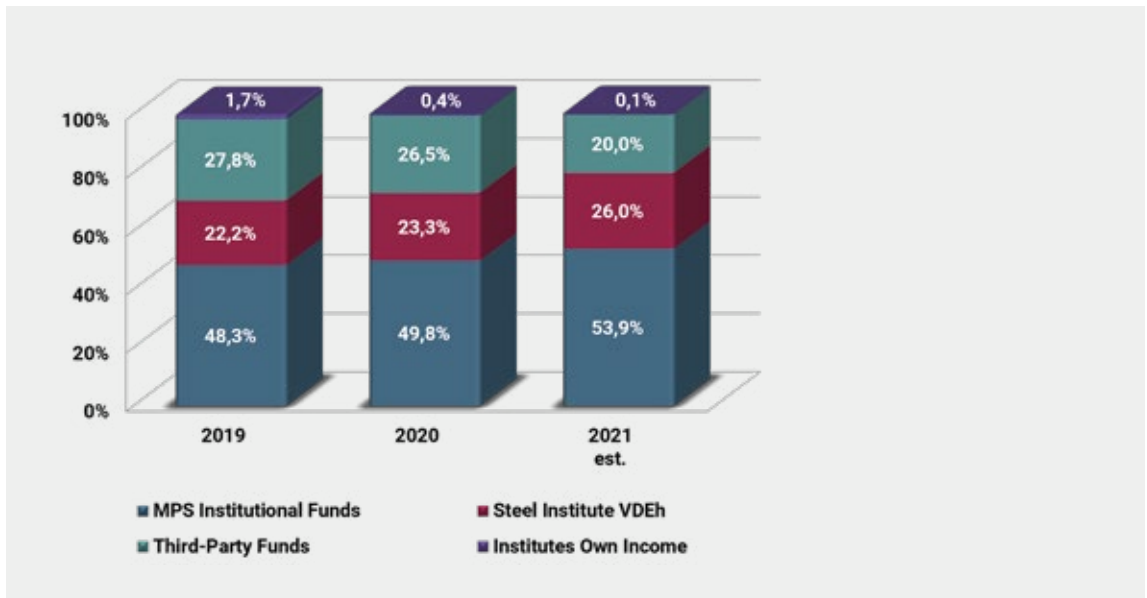
Member National Academy Leopoldina, 2013

Honorary Professor at Katholieke Universiteit Leuven, Belgium, 2014

Budget of the institute

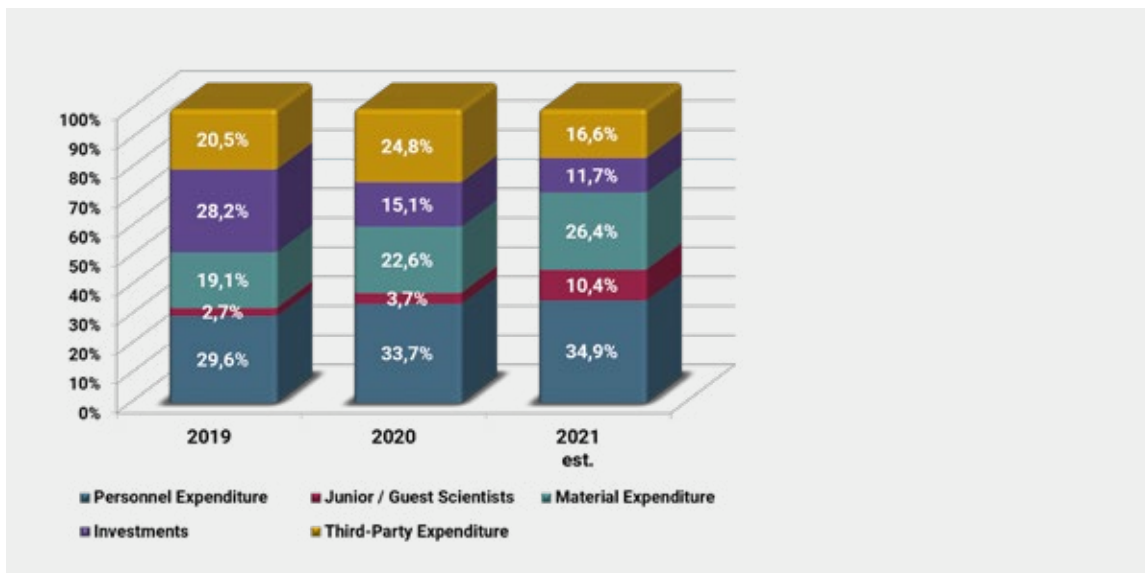
Revenue

(Percentual contributions to total revenue without appointment-related investment funds and general reconstruction of the buildings; year 2021 data estimated)



Expenditure

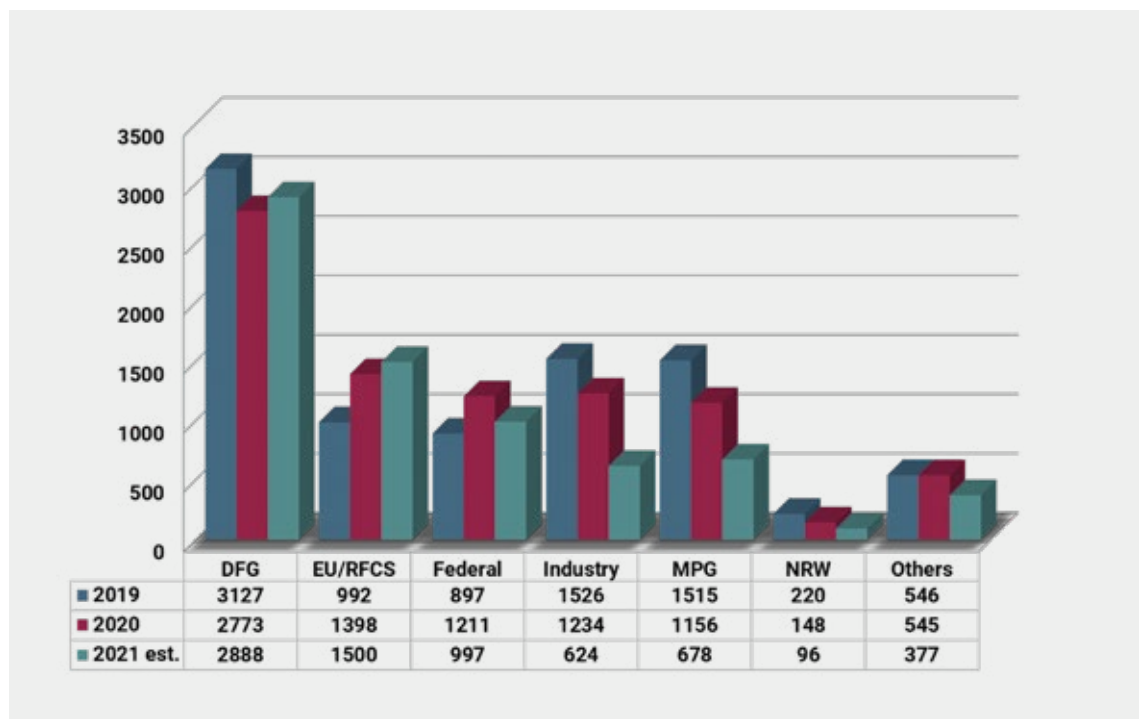
(Percentual distribution of total expenditure; investments include large-scale apparatus, electronic data processing, appointment-related investments, separate investment for basic equipment; year 2021 data estimated)





Third-party funds

(Contributions in 1,000 € to total revenue including personnel, material and investments, year 2021 data estimated)



DFG: German Science Foundation

EU: European Union

RFCS: Research Fund for Coal and Steel

Federal: BMBF & BMWi

BMBF: Federal Ministry of Science and Education

BMWi: Federal Ministry of Economics and Technology

Industry incl. Christian Doppler Society and MaxNet

MPG: Max Planck Society

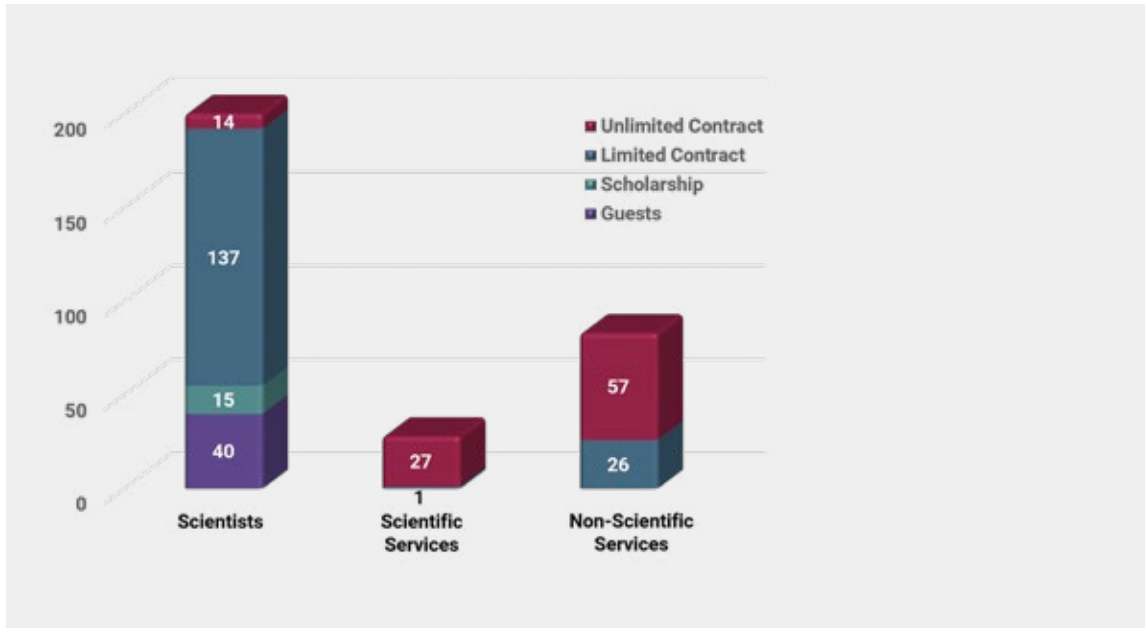
NRW: State of North Rhine-Westphalia

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

Personnel structure

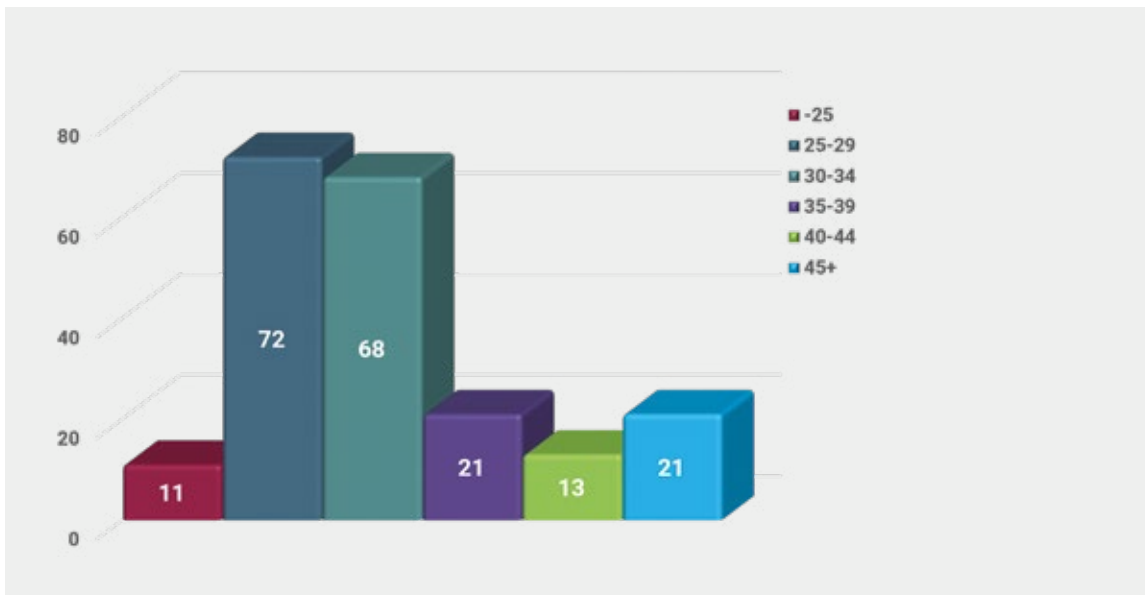
Number of occupied scientific / non-scientific positions

(Absolute numbers, September 2021)



Age distribution of junior scientists

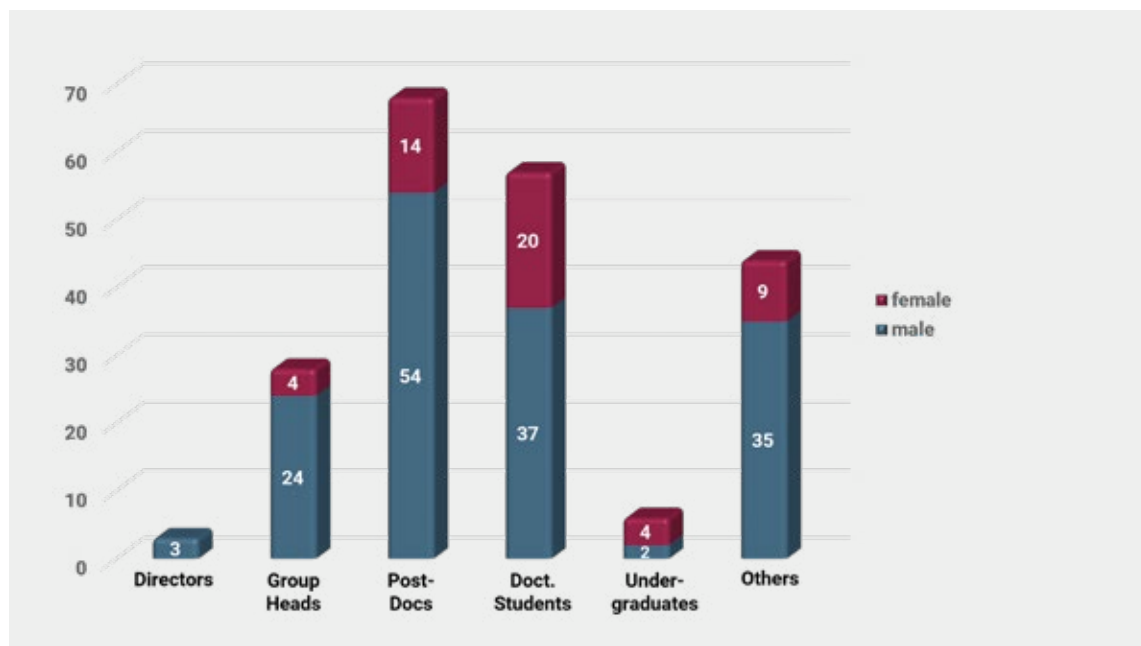
(Absolute numbers, September 2021)





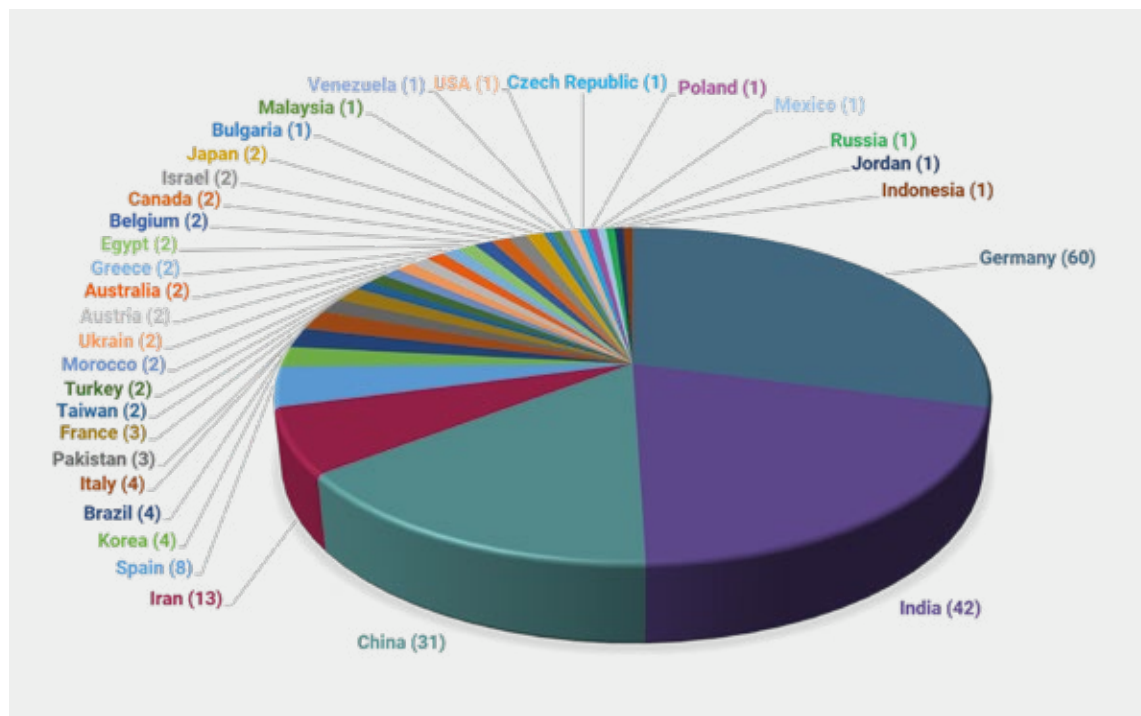
Gender distribution of scientists

(Absolute numbers, September 2021)



Scientists and their home countries

(Absolute numbers, September 2021)

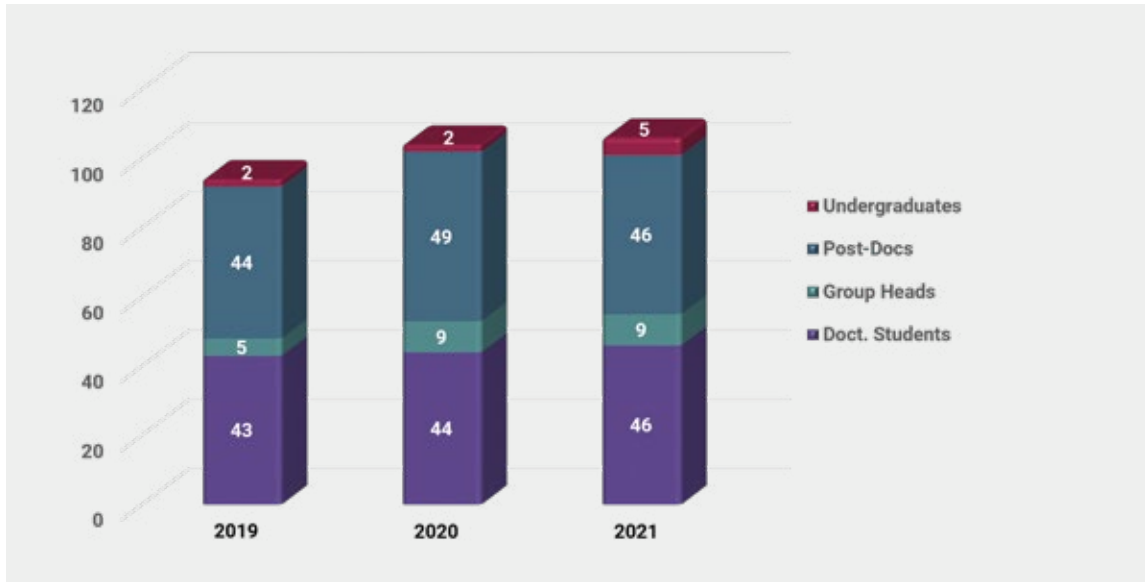




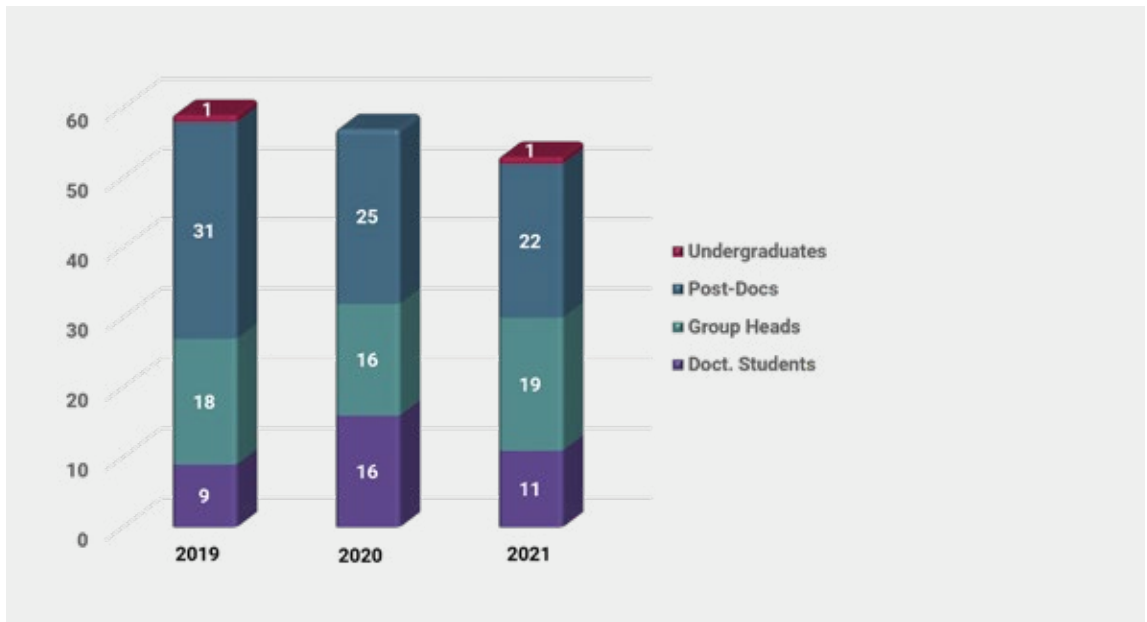
Number of junior scientists

(Absolute numbers, year 2021 data estimated)

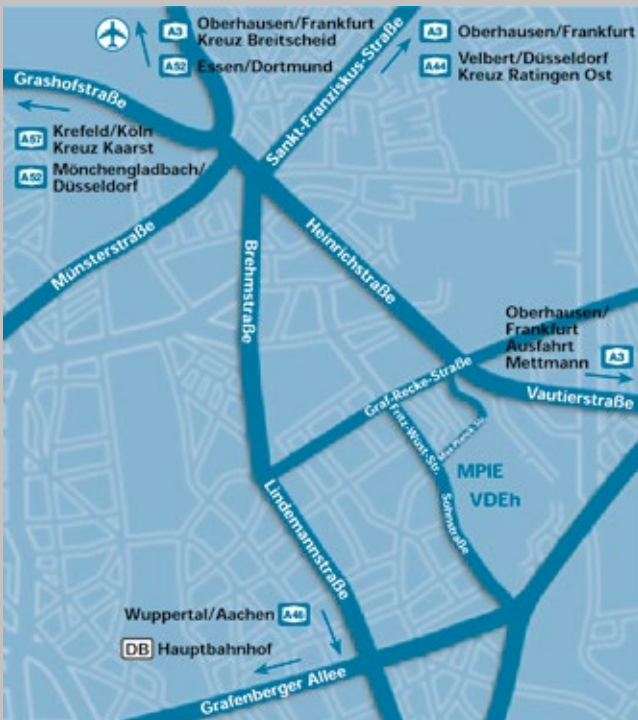
Financed via third-party funds



Not financed via third-party funds



Scientific Report 2019 – 2021



Max-Planck-Institut für Eisenforschung GmbH

Max-Planck-Straße 1
D-40237 Düsseldorf

Phone: +49-211-6792-0

Fax: +49-211-6792-440

Homepage: <https://www.mpie.de>

Access

from Central Railway Station:

by Bus 834 (direction Belsenplatz)
to stop Sohnstraße

by Taxi to Sohnstraße/Max-Planck-Straße,
10 minutes

from Airport:

by Taxi to Sohnstraße/Max-Planck-Straße,
15 minutes