



PART IV.

GENERAL INFORMATION AND STATISTICS

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Boards, Directors, Max Planck Fellows, External Scientific Members and Guest Scientists

Supervisory Board (as of January 2019)

Prof. Dr. Ferdi SCHÜTH (Chairman 2019/2020)
Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V., München

Hans Jürgen KERKHOFF (Vice-Chairman 2019/2020)
Stahlinstitut VDEh, Düsseldorf

Martin BAUES
Saarstahl AG, Völklingen

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

Dr.-Ing. h.c. Hans FISCHER
Tata Steel Europe Ltd., IJmuiden, The Netherlands

Dr. Heribert R. FISCHER
thyssenkrupp Steel Europe AG, Duisburg

Staatssekretärin Annette STORSBERG
Ministerium für Kultur und Wissenschaft des Landes Nordrhein-Westfalen, Düsseldorf

Univ.-Prof. Dr. Ulrich RÜDIGER
Rheinisch-Westfälische Technische Hochschule Aachen, Aachen

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

RD Dr. Peter SCHROTH
Bundesministerium für Bildung und Forschung: Schlüsseltechnologien für Wachstum, Bonn



Scientific Advisory Board (as of January 2019)

Prof. Dr. Hans FERKEL

thyssenkrupp Steel Europe AG, Duisburg

Prof. Dr. Peter GUMBSCH

Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg

Prof. Dr. Wolfgang JÄGER

Christian-Albrechts-University (CAU) zu Kiel, Kiel

Dr. Juliane MENTZ

Salzgitter Mannesmann Forschung GmbH, Duisburg

Prof. Dr. Michael John MILLS

Ohio State University, Columbus, USA

Prof. Dr. George PHARR

Texas A&M University, College Station, USA

Prof. Dr. Tresa M. POLLOCK

University of California, Santa Barbara, USA

Prof. Dr. Mary P. RYAN

Imperial College London, London, UK

Dr. André SCHNEIDER

Vallourec Deutschland GmbH, Düsseldorf

Dr.-Ing. Michael STEINHORST

Tata Steel R&D, Ijmuiden, the Netherlands

Dr. Alois STREISSELBERGER

AG der Dillinger Hüttenwerke, Dillingen

Prof. Dr. Adrian SUTTON

Imperial College London, London, UK

Prof. Dr.-Ing. A. Erman TEKKAYA,

Technische Universität Dortmund, Dortmund

Prof. Dr. Herman TERRYIN

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 22nd Sept. 2015)

Max Planck Fellow:

Prof. Jochen M. SCHNEIDER, Ph.D., RWTH Aachen University (since Oct. 2015)

External Scientific Members:

Prof. Dr. Mats HILLERT, Stockholm, Sweden

Prof. Dr. Reiner KIRCHHEIM, Göttingen



Guest Scientists

Alexander von Humboldt-Foundation

Dr. Andrew Breen (Australia), University of Sydney/AU, Humboldt Research Fellowship for Postdoctoral Researchers; Jun 2018 to May 2020

Dr. Chang Hyuck Choi (Korea), Korea Advanced Institute of Science and Technology/KR, Humboldt Research Fellowship for Postdoctoral Researchers; May 2015 to Apr 2017

Dr. Haidong Fan (China), Sichuan University/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Sep 2017 to Aug 2018

Dr. Xufei Fang (China), Tsinghua University/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Oct 2016 to Aug 2018; Oct 2018 to Sep 2019

Prof. Dr. Mike Finnis (UK), Imperial College London/UK, Humboldt Research Award; Aug to Sep 2016; Jul 2017; Jul to Aug 2018

Dr. Raheleh Hadian (Iran), McMaster University/CA, Humboldt Research Fellowship for Postdoctoral Researchers; Mar 2015 to Feb 2017

Dr. Jeongho Han (Korea), Yonsei University/KR, Humboldt Research Fellowship for Postdoctoral Researchers; Apr 2016 to Aug 2018

Dr. Luo Hong (China), University of Science and Technology/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Jan 2016 to Dec 2017

Dr. Rong Hu (China), Tsinghua University/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Aug 2014 to Jul 2016

Dr. Lim Joohyun (Korea), Ewha Womans University/KR, Humboldt Research Fellowship for Postdoctoral Researchers; Mar 2018 to Apr 2020

Dr. Olga Kasian (Ukraine), Ukraine State University of Chemical Technology/UA, Humboldt Research Fellowship for Postdoctoral Researchers; Apr 2015 to Mar 2017

Dr. Jinkyung Kim (Korea), Pohang University of Science and Technology (POSTECH)/KR, Humboldt Research Fellowship for Postdoctoral Researchers; Jun 2013 to Feb 2016

Dr. Dong-Hyun Lee (Korea), Hanyang University/KR, Humboldt Research Fellowship for Postdoctoral Researchers; Nov 2018 to Oct 2020

Dr. Jianjun Li (China), Northwestern Polytechnical University/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Jun 2015 to May 2017

Dr. Jiehua Li (China), Northwestern Polytechnical University/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Jun to Sep 2018; Jun to Sep 2019; Jun to Sep 2020

Dr. Linlin Li (China), University of Shenyang/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Feb 2018 to Jan 2020

Dr. Tong Li (China), Beijing University/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Mar 2016 to Nov 2017

Dr. Surenda Kumar Makineni (India), Indian Institute of Science, Bangalore/IN, Humboldt Research Fellowship for Postdoctoral Researchers; Jun 2017 to May 2019

Prof. Roger Reed (UK), University of Oxford/UK, Humboldt Research Award; since Nov 2012

Prof. Paulo Rios (Brazil), Universidade Federal Fluminense (UFF)/BR, Humboldt Research Award; Dec 2015 to Feb 2016

Dr. Seok Su Sohn (Korea), Pohang University of Science and Technology (POSTECH)/KR, Humboldt Research Fellowship for Postdoctoral Researchers; Jul 2017 to Jan 2019

Dr. Binhan Sun (China), Northeastern University/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Mar 2018 to Feb 2020

Dr. Sai Tang (China), Northwestern Polytechnical University/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Jan 2016 to Dec 2017

Dr. Michael Titus (USA), University of California/US, Humboldt Research Fellowship for Postdoctoral Researchers; Dec 2015 to Nov 2017

Dr. Zhangwei Wang (China), Central South University/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Nov 2017 to Oct 2019

Dr. Fengkai Yan (China), Institute of Metal Research, Chinese Academy of Sciences/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Apr 2017 to Mar 2019

Prof. Yao Yao (China), Northwestern Polytechnical University/CN, Humboldt Research Fellowship for Experienced Researchers; Sep 2018 to Aug 2019

Dr. Yifan Ye (China), City University of Hong Kong/CN, Humboldt Research Fellowship for Postdoctoral Researchers; May 2018 to Apr 2020

Dr. Xu Zhang (China), Southwest Jiaotong University/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Sep 2016 to Aug 2018

Dr. Xiankang Zhong (China), State Key Laboratory of Oil and Gas/CN, Humboldt Research Fellowship for Postdoctoral Researchers; Sep 2016 to Aug 2017

Kahl Zilnyk, M.Sc. (Brazil), Escola de Engenharia de Lorena, University of São Paulo (EEL-USP)/BR, Humboldt Research Fellowship for Postdoctoral Researchers; Dec 2015 to Feb 2016

German Academic Exchange Service (DAAD)

Shih-Che Chen, B.Sc. (Taiwan), MOST (Ministry of Science and Technology)/DAAD Taiwan Summer Institute/TW 2017; Jul to Sep 2017

Dr. Ying-Hsuan Chen (Taiwan), Academia Sinica/TW; Oct 2014 to Sep 2017

Guang-Ju Cheng (Taiwan), MOST (Ministry of Science and Technology)/TW; Sep 2018 to Apr 2019

Won-Seok Choi, M.Sc. (Korea), Pohang University of Science and Technology (POSTECH)/KR, German Academic Exchange Service (DAAD); Apr 2015 to Mar 2016; Oct 2016 to Jan 2018

Dr. Viacheslav Shkirskiy (Russia), Chimie Paris Tech/F; Mar to Jun 2017

Prof. Dr. Ricardo Manuel Souto Suarez (Spain), University La Laguna/ES; Jun to Jul 2017

Diverse Guest Scientists

Sehar Abbas, B.Sc. (Pakistan), Mehran University/ PK; Feb 2016 to Apr 2016

Kohei Abe (Japan), Hokkaido University of Science/ JP; Feb to Mar 2016; Aug 2016

Dr. Björn Alling (Sweden), Linköping University/SE, Sep 2017; Oct 2017; Dec 2017; Jan 2018; Feb 2018; Jun 2018

Prof. Yaron Amoyal (Israel), Technion – Israel Institute of Technology/IL; Aug 2018

Leonardo Shoji Aota, M.Sc. (Brazil), Escola de Engenharia de Lorena, University of São Paulo (EEL-USP)/BR; Sep 2017 to Feb 2018

Raquel Aymerich Armengol (Spain), Universitat Autònoma de Barcelona/ES; Feb to Jun 2018

Dr. Theodoros Baimpos (Greece), University of Patras/GR, Postdoctoral Fellow; Jan to Jun 2016

Prof. Jayasundera Bandara (Sri Lanka), Institute of Fundamental Studies/LK; Jul to Sep 2016

Pierre Beley (France), Polytech Lyon/F, Erasmus exchange student; Mar to Sep 2017

Dr. Sedigheh Bigdeli (Iran), Royal Institute of Technology/SE, Sep 2015 to Oct 2015

Tyler B. Blum, M.Sc. (USA), University of Madison/ US; Jan to Feb 2018

Carsten Bonnekoh, M.Sc. (Germany), Karlsruhe Institute of Technology (KIT)/DE; Mar to May 2017

Prof. Limei Cha (China), College of Materials Science and Engineering, Hunan University/CN; Jun to Jul 2017

Assoc. Prof. Jay Chakraborty (India), National Metallurgical Laboratory/IN; Feb to Jun 2016

Yanhong Chang, M.Sc. (China), Sichuan University/ CN, China Scholarship Council (CSC); Oct 2015 to Sep 2019

Dr. Dominique Chatain (France), Aix-Marseille Université, CINaM (CNRS)/FR; Jul 2017

Ran Chen, B.Sc. (China), Shanghai Jiao Tong University (SJTU)/CN, China Scholarship Council (CSC); Feb 2015 to Jan 2017

Dr. Serhiy Cherevko (Ukraine), Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN) /DE, Postdoctoral Research Fellow; Dec 2011 to Aug 2018

Dr. Wonseok Choi (Korea), Korean Institute of Science & Technology (KAIST)/KR; Jul to Aug 2018

Ning Dang, M.Sc. (China), Baihang University/CN; Nov 2017 to Jan 2018

Farnaz Abdollahzadeh Davani, M.Sc. (Iran), University of Sistan and Baluchestan/IR; Feb 2017 to Feb 2019

Dr. Palanisamy Dhanalakshmi (India), Indian Institute of Science, Bangalore/IN; Apr 2017 to Apr 2018

Raphael Engel (France), Grenoble INP/FR; May to Jul 2018

Machmut Ersani, M.Sc. (Turkey), Ruhr Universität Bochum/DE; Apr 2017 to Apr 2018

Dr. Loïc Exbrayat (France), Université de La Rochelle/FR, Postdoctoral Fellow; Jan to Mar 2016

Isnaldi Rodrigues de Souza Filho, M.Sc. (Brazil), Escola de Engenharia de Lorena, University of São Paulo (EEL-USP)/BR; Oct 2017 to Sep 2018

Jorge Luis Martins Guerra Filho, M.Sc. (Brazil), Universidade Federal do Rio de Janeiro (UFRJ)/ BR; May 2017 to Apr 2020

Axel Forslund (Sweden), Royal Institute of Technology/SE; May to Jun 2018

Guilherme Vilalba Fortunato, M.Sc. (Brazil), Universidade Federal de Mato Grosso do Sul/BR; Jul 2017 to Jun 2018

Dr. Martin Friák (Czech), Institute of Physics of Materials of the Academy of Sciences of the Czech Republic (IPM Brno)/CZ; Dec 2016; Feb 2017; Oct 2017; Jun 2018

Noriki Fujita, M.Sc. (Japan), JFE Steel Corporation, Fukuyama/JP; Sep 2013 to Dec 2015



Dr. Junying Hu (China), State Key Laboratory of Oil and Gas/CN, Chinese Scholarship Council; Sep 2016 to Sep 2017

Dr. Pradeep Konda Gokuldoss (India), RWTH Aachen University/DE; May 2014 to Apr 2018

Dr. Mark Greiner (Canada), MPI für Chemische Energiekonversion, Mülheim a.d.R./DE; Jul to Aug 2018

Dr. James Griffiths (UK), Cambridge/UK; Apr 2016

Yueling Guo, M.Sc. (China), Beihang University/CN, Chinese Scholarship Council (CSC); Oct 2017 to Sep 2019

Dr. Ivan Gutierrez-Urrutia (Spain), Research Center for Strategic Materials, National Institute for Materials Science/JP; Jul 2017

Dr. Masood Hafez (Iran), VDM Metals GmbH/DE; Feb 2015 to Dec 2016

Michael Haines, B.Sc. (USA), University of Tennessee/US; Jan to Jul 2018

Dr. Nima Hamidi (Iran), Institut für Theoretische Physik, AG Computersimulationen und Theorie komplexer Fluide, TU Berlin/DE; Feb 2015 to Jan 2016

Ian Harding, M.Sc. (USA), Brown University/US; May to Jun 2018

Dr. Jinshan He (China), Beijing University/CN; Jul to Aug 2018

Anders Holten (Denmark), University of Copenhagen/DK, Visiting Researcher; Nov 2015 to Apr 2016

Prof. Toshiaki Horiuchi (Japan), Hokkaido University of Science/JP; Feb to Mar 2016; Aug 2016; Oct 2017; Aug 2018

Dr. Junying Hu (China), State Key Laboratory of Oil and Gas/CN, Chinese Scholarship Council; Sep 2016 to Sep 2017

Dr. Qingyun Hu (China), Ruhr University Bochum/DE, RESOLV Fellow; Mar 2014 to Aug 2018

Mingda Huang, M.Sc. (China), Xi'an Jiaotong University/CN, Chinese Scholarship Council (CSC); Oct 2017 to Sep 2019

Dr. Yuji Ikeda (Japan), Kyoto University/JP; Mai 2017 to Apr 2018

Hyeji Im, M.Sc. (Korea), Korean Institute of Science & Technology (KAIST), Seoul/KR; Jul 2017 to Feb 2018

Dr. Shoji Ishibashi (Japan), National Institute of Advanced Industrial Science and Technology/JP; Feb 2018; Mai to Oct 2018

Prof. Balila Nagamani Jaya (India), Indian Institute of Technology Bombay/IN; May to Jun 2017, Jul 2018

Dr. Darja Jenko (Slovenia), Institute of Metals and Technology (IMT)/SI; Jul 2017 to Jul 2018

Hosun Jun, B.Sc. (Korea), Korean Institute of Science & Technology (KAIST), Seoul/KR; Jun 2018 to Jan 2019

Dr. Reza Darvishi Kamachali (Iran), Tehran University, Tehran/IR; Heisenberg Fellowship; Feb 2018 to Jan 2021

Sho Katsura, M.Sc. (Japan), Kobe Steel/JP; Oct 2017 to Sep 2018

Mehrin Peyman Khanipour, M.Sc. (Iran), Forschungszentrum Jülich/DE; Aug 2016 to Jul 2017

Dr. Jong-Hee Kim (Korea), POSCO (Pohang Iron and Steel Company)/KR; Dec 2017 to Dec 2018

Julius Knöppel, M.Sc. (Germany), Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN) /DE; Dec 2017 to Dec 2018

Peter Konijnenberg, Dipl.-Ing. (The Netherlands), Bruker Nano GmbH, Berlin/DE; Jan 2014 to Dec 2018

Assist. Prof. Dr. Maciej Krzwiecki (Poland), Silesian University of Technology/PL; several short-term research visits; 2012 to 2018

Ankit Kumar, M.Sc. (India), Indian Institute of Technology Roorkee/IN, TU Delft /NL; Nov 2015 to Jul 2017

Dr. Alisson Kwiatkowski da Silva (Brazil), Universidade Estadual de Ponta Grossa, UEPG (State University of Ponta Grossa)/BR, Brazilian Government (Science Without Borders); Apr 2015 to Sep 2018

Dr. Minjie Lai (China), Northwestern Polytechnical University, Xi'an/CN, China Scholarship Council (CSC); Aug 2012 to Aug 2016

Dr. Christopher Laursen (USA), University of Wyoming/US; Jan to Apr 2018

Juan Li, M.Sc. (China), University of Science and Technology Beijing/CN; since Oct 2015

Zhuangming Li, M.Sc. (China), University of Science and Technology Beijing (USTB)/CN; Jul to Oct 2018

Chuanlai Liu, M.Sc. (China), Shanghai Jiao Tong University/CN, China Scholarship Council (CSC); Oct 2015 to Sep 2017; Feb 2018

Andreas Lücke (Germany), Universität Paderborn/DE, for research exchange; Jan to May 2016

Wei Luo, M.Sc. (China), Central South University/CN, China Scholarship Council (CSC); Nov 2014 to Oct 2017

Caleb Massey, M.Sc. (USA), University of Tennessee/US; Oct to Nov 2017

Nidhin George Mathews (India), Indian Institute of Technology Bombay/IN; Jul 2018

Sami Meddeb, B.Sc. (Tunisia), PHELMA, Grenoble (INP)/FR; May to Jul 2018

Prof. Sai Ramudu Mekka (India), Indian Institute of Technology Roorkee/IN, MPG-DST Partner Group; Mar 2017 to Feb 2020

Maisam Merali (UK), University of Cambridge/UK; Jul to Aug 2018

Dr. Stefano Mezzavilla (Italy), Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN)/DE; Jan to Dec 2016

Dr.-Ing. Jaber Rezaei Mianroodi (Iran), Sharif University of Technology/IR; Nov 2017 to Dec 2019

Dr. Boaz Moeremans (Belgium), Hasselt University/BE; Jan to Dec 2016

Jesús Salvador Mondragón Ochoa, M.Sc. (Mexico), University of Guanajuato/MX, CONACYT Doctoral Fellowship; Oct 2013 to Jun 2018

Jacob Monroe, M.Sc. (USA), University of California/US; Jan to Dec 2016

Dr. Igor Moravčík (Czech Republic), Brno University of Technology/CZ; Feb to Apr 2018; Sep 2018 to Feb 2019

Andres Felipe Jaramillo Muñoz, M.Sc. (Colombia), Universidad de Concepción/CO; Mar to May 2018

Fang Niu, M.Sc. (China), Ruhr Universität Bochum/DE; Jun 2016 to Sep 2017

Niklas Osterloh (Germany), Ruhr Universität Bochum/DE; Jan to Dec 2016

Beibei Pang, M.Sc. (China), Ruhr Universität Bochum/DE; Jul 2014 to Dec 2017

Dr. Yuan Ping (China), University of California/US; Jan to Dec 2016

Dr. Ivan Postugar (Russia), Forschungszentrum Jülich/DE; Jan 2016 to Dec 2018

Dr. Sangeetha Raman (India), Indian Institute of Technology Madras/IN; Jan to Dec 2016

Andrea Valencia Ramirez (Mexico), Center for Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV)/MX; Apr to Jul 2018

Davison Ramos de Almeida Junior, M.Sc. (Brazil), Universidade de São Paulo (EEL-USP)/BR; May to Oct 2017

Ziyuan Rao, M.Sc. (China), Beijing University/CN, China Scholarship Council (CSC); Sep 2017 to Aug 2021

Adam Ready (UK), Imperial College London/UK, May 2015; Nov to Dec 2015

Nicolás A. Rivas, M.Sc. (Venezuela), Simón Bolívar University (Caracas)/VE, University of Ghent/BE; Mar 2015 to Dec 2018

Dr. Kristiane Ann Kathrin Rusitzka (Germany), Max-Planck-Institut für Eisenforschung/DE, Experiment!-Fellow (VW Foundation); Jun 2017 to Jun 2018

Dr. Ryoji Sahara (Japan), National Institute for Materials Science/JP, Jul 2015 to Jun 2016

Dr. Maria Samdim (Brazil), Universidade de São Paulo (EEL-USP)/BR; Apr 2016; Jun 2017; Mar 2018

Daniel Sandbeck, M.Sc. (Germany), Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN)/DE; Aug 2016 to Jul 2017

Prof. Hugo Sandim (Brazil), Universidade de São Paulo (EEL-USP)/BR; Apr 2016; Jun 2017; Mar 2018

Dr. Vitalij Schmidt (Germany), Münster University/DE; Mar 2016 to Mar 2017

Anton Schneider (France), CEA Saclay/FR; Jan 2018

Dr. Torsten Schwarz (Germany), RWTH Aachen University/DE; Sep 2015 to Apr 2016

Kai Alexander Schwenzfeier, M.Sc. (Germany), TU Wien/AT; Jul 2015 to Nov 2018

Dr. Karo Sedighiani (Iran), TU Delft/NL; Apr 2017 to Mar 2020

Javiera Aguirre Sepúlveda, M.Sc. (Chile), Pontificia Universidad Católica de Chile/CL; Jan to Jul 2018

Andreja Šestan (Slovenia), Jožef Stefan Institute (JSI)/SI; Aug 2017 to Aug 2018

Dr. Pratheek Shanthraj (India), North Carolina State University/US; Aachen Institute for Advanced Study in Computational Engineering Science (AICES); Jun 2014 to May 2016; Jun 2018 to May 2020

Dr. Alexander Shapeev (Russia), Skoltech, Stolkovo Innovation Center/RU, Apr 2018

Ariel Sheskin, B.Sc. (Israel), Technion/IL; Minerva Scholarship; Aug 2016 to Sep 2016

Dr. Reinhard Sigel (Germany), German University in Cairo (GUC)/EG; Feb to Dec 2017

Gabriel da Silva, Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN)/DE; Dec 2017 to Dec 2018

Dr. Sanjay Singh (India), Max-Planck-Institut für Chemische Physik fester Stoffe/DE; Jul 2016

Dr. Michaela Šlapáková (Czech Republic), Charles University Prague/CZ; Sep 2015 to Aug 2016; Mar to Apr 2017



- Purvesh Soni*, M.Sc. (India), RWTH Aachen University/DE; Sep 2015 to Aug 2018
- Florian Speck*, M.Sc. (Germany), Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN)/DE; Jan to Jul 2017
- Prashanth Srinivasan* (India), TU Delft/NL, Apr 2018; Oct 2018; Dec 2018
- Dr. Irina Stockem* (Germany), Linköping University/SE, Aug 2016 to Feb 2017, Aug 2018 to Jul 2019
- Dr. Andreas Stoffers* (Germany), RWTH Aachen University/DE; Sept 2015 to Aug 2016; Jan to Jun 2017
- Prof. Bob Svendsen* (USA/Germany), RWTH Aachen University/DE; cooperation with RWTH Aachen University; since Mar 2012
- Dr. Agnieszka Szczepaniak* (Poland), Wrocław University/PL; Jan to Jun 2018
- Haleh Taghinejadi* (UK), University of Cambridge/UK; Jul to Aug 2017
- Chris Talbot* (UK), University of Cambridge/UK; Jul to Aug 2018
- Xiaodong Tan*, M.Sc. (China), Northeastern University, Shenyang/CN, China Scholarship Council (CSC); Oct 2015 to Sep 2016
- Komomo Tani* (Japan), Advanced Technology Research Laboratories, Nippon Steel & Sumitomo Metal Corporation/JP; Jul 2016 to Jun 2018
- Dr. Shunsuke Taniguchi* (Japan), Advanced Technology Research Laboratories, Nippon Steel & Sumitomo Metal Corporation/JP; May 2016 to Apr 2017
- Stefanie Tecklenburg*, M.Sc. (Germany), Ruhr Universität Bochum/DE; Jan 2016 to Jan 2018
- Katie Tidd* (UK), University of Cambridge/UK; Jul to Aug 2017
- Konstantina Traka*, M.Sc. (Greece), National Technical University of Athens/GR, TU Delft/NL; Jul 2017 to Jun 2019
- Dr. Mizuki Tsuboi* (Japan), Kyoto University/JP; Jul 2017 to Aug 2018
- Daniel Varley* (UK), University of Cambridge/UK; Jul to Aug 2016
- Ruben Bueno Villoro* (Spain), Universitat Autònoma de Barcelona/ES; Jul to Aug 2017; Feb to Jun 2018
- Lixiao Wang*, M.Sc. (China), Tsinghua University/CN, China Scholarship Council (CSC); Mar 2016 to Aug 2016
- Dr. Xiaoxiang Wu* (China), Ruhr Universität Bochum/DE, Apr 2017 to Dec 2018
- Dr. Yun Wu* (China), Shanghai University/CN; Jan to Aug 2018
- Jinghua Xin* (China), Central South University/CN, Sep 2015 to Sep 2016
- Konatsu Yamada* (Japan), Hokkaido University of Science/JP; Aug 2018
- Suhyun Yoo* (Korea), Ruhr Universität Bochum/DE; Mar 2016 to Feb 2018
- Kooknoh Yoon*, M.Sc. (Korea), Seoul National University/KR, Scholarship of 'Research Exchange Program' between Korea and ERC (EU); Sep 2018 to Aug 2019
- Dr. Janez Zavašnik* (Slovenia), Jožef Stefan Institute (JSI)/SI; Aug 2017 to Aug 2018
- Dr. Han Zhang* (China), Tsinghua University, Beijing/CN; Jan to Jun 2016
- Dr. Jian Zhang* (China), Xi'an Jiaotong University/CN; Apr to Jul 2018
- Jiecen Zhang*, M.Sc. (China), Northeastern University, Shenyang/CN, China Scholarship Council (CSC); Oct 2015 to Sep 2016
- Huan Zhao*, M.Sc. (China), Chongqing University/CN, China Scholarship Council (CSC); Oct 2014 to Sep 2019
- Tian Rong Zhu* (UK), University of Cambridge/UK; Jul to Aug 2016



Scientific Honours

2015 (not included in the Scientific Report 2013 - 2015)

Prof. Dierk Raabe was awarded the Certificate of Excellence in Reviewing from Acta Materialia & Elsevier in recognition of significant contributions made to the quality of the journal, 2015

Prof. Paulo Rangel Rios from Universidade Federal Fluminense (UFF), Rio de Janeiro (Brazil) has been awarded a Return Fellowship of the Humboldt Research Award, Dec 2015

Dr. Franz Roters became member of the Editorial Board of Philosophical Magazine and Philosophical Magazine Letters, Oct 2015

Dr. Cem Tasan former leader of the group Adaptive Structural Materials (until Dec 2015) won the Freigeist Fellowship of the Volkswagen Foundation, Jun 2015

Dr. Markus Valtiner was elected as member-at-large for the Biointerfaces Division of the American Vacuum Society, Oct 2015

Dr. Markus Valtiner received an ERC Starting Grant for the project “CSI.interface - A molecular interface science approach: Decoding single molecular reactions and interactions at dynamic solid/liquid interfaces”, Dec 2015

Ali Zendegani received the Larry Kaufman Scholarship 2015 to present his research on “First-principles study of thermodynamic properties of the Q phase in Al-Cu-Mg-Si” at the CALPHAD XLIV conference, Loano (Italy), May 2015

2016

Christian Broß has been honoured by the Chamber of Industry and Commerce (IHK) Düsseldorf being one of the Best Trainees 2016, Oct 2016

Christian Broß won the Max Planck Trainee Prize by the Max Planck Society, one of the best trainees of all Max Planck Institutes, Sep 2016

Christian Broß received the 1st Poster Award at the Conference Mikpräg 2015, Solingen (Germany) with his poster “Study of New Methods to Analyse Chromium-Nickel Steels”, Jun 2016

Dr. Vijayshankar Dandapani was selected to give an invited talk at the Gordon Research Conference 2016 on Aqueous Corrosion, New London (USA), Jul 2016

Dr. Martin Diehl received the Deutsche Gesellschaft für Materialkunde e.V. (DGM) – Nachwuchspreis, Sep 2016

Dr. Andreas Erbe and Dr. Michael Auinger received the Best Paper Award for the years 2014 - 2015 from EOS (Journal of the European Optical Society) for their paper “Effect of surface roughness on optical heating of metals”, Sep 2016

Herbert Faul was lent the honorary needle in silver with thanks and recognition for his 10 years honorary engagement in professional training by Niederrheinische Industrie- und Handelskammer, Duisburg-Wesel-Kleve (Germany), Aug 2016

Dr. Martin Friák, Dr. Stefanie Sandlöbes, Z. Pei, Dr. Duangcheng Ma, Prof. Bob Svendsen, Prof. Dierk Raabe and Prof. Jörg Neugebauer won one of three poster prizes with the poster “An ab initio high throughput approach to identify MG-alloys with exceptionally high yield strength” at the 80th Annual Meeting of the German Physical Society (DPG) in Regensburg (Germany). The shown results are based on a close interdisciplinary work between scientists of the two departments “Computational Material Design” and “Microstructure Physics and Alloy Design”, Mar 2016

Dr. Baptiste Gault was awarded the Volkswagen Foundation ‘Experiment!’ research project on “Enabling atomic-scale tomography of biological material”, Oct 2016



Dr. Michael Herbig received 1.468 Mio € funding by the BMBF for his junior research group “Materials Science of Mechanical Contacts”, Sep 2016

Stefan Hieke received a Travel Award from the DGE (Deutsche Gesellschaft für Elektronenmikroskopie) to participate at the European Microscopy Conference EMC 2016 in Lyon (France) Sep 2016

Dr. Nejc Hodnik got a Marie-Curie Intra-European Fellowship „EIWBinsTEM - Development of electrochemical water based in-situ TEM and study of platinum based nanoparticles potential- and time-dependent changes“, Apr 2014 to Mar 2016

Dr. Motomichi Koyama, Dr. Asif Bashir and PD Dr. Michael Rohwerder received the Japan Institute of Metals and Materials Metallography Award (Fine work prize), Mar 2016

Nataliya Malyar received one of two prestigious Best Poster Awards at the Gordon Research Conference 2016 in Lewiston, Maine (USA), Aug 2016

Prof. Jörg Neugebauer was awarded the 2015 Ernst Mach Medal of the Czech Academy of Sciences, May 2016

Julian Rechmann obtained a Best Poster Award at the 16th International Conference on Organized Molecular Films (ICOMF16), Helsinki (Finland), Jul 2016

Dr. Hauke Springer, Dr. Cem Tasan and Prof. Dierk Raabe received the Werner Koester Award for the paper “A novel roll bonding methodology for the cross-scale analysis of phase properties and interactions in multiphase structural materials” published in IJMR 106 (2015), 3-14, Sep 2016

Dr. Frank Stein and Irina Wossack received the Best Paper Award of the Alloy Phase Diagram International Commission for the year 2015, Jul 2016

Daniel Varley won the 2016 European Placement Prize of the University of Cambridge for his work on high-temperature polymer electrolyte membrane fuel cells, which he performed during his two-month summer internship in the independent research group of Prof. Christina Scheu, Nov 2016

Dr. Aleksandar R. Zeradjanin was selected to give an invited lecture at the 67th Annual Meeting of the International Society of Electrochemistry (ISE) and was invited to chair the session at the Symposium: “Novel Materials and Devices for Energy Conversion and Storage”, Haag (The Netherlands), Aug 2016

2017

Priyanshu Bajaj received the Best Poster Award: ADDMAT conference, Tiruvananthapuram (India), Dez 2017

Janine Birnbach received the Apprentice Prize for one of the best final exams in the profession of laboratory technician, Chamber of Industry and Commerce (IHK) Düsseldorf (Germany), Oct 2017

Heidi Bögershausen and Luca Bender gained the 2nd poster prize at the „Fachtagung für Mikroskopie und Präparation (MikPräp) 2017“, Solingen (Germany) with their poster about „Haushalts- und Lebensmittel als alternative Ätzmethode“, Apr 2017

Dr. Martin Diehl, Christian Broß and Prof. Dierk Raabe won the 3rd poster prize with the poster „Quasi in situ Untersuchung der statischen Rekristallisation in DC 04 Stahl“ at the „Fachtagung für Mikroskopie und Präparation (MikPräp) 2017“, Solingen (Germany), Apr 2017

Till Freieck won the Max Planck Trainee Prize by the Max Planck Society, one of the best trainees of all Max Planck Institutes, Aug 2017

Dr. Blazej Grabowski received the Acta Journals Outstanding Review Award for 2016, Apr 2017

Dr. Michael Herbig has been awarded the Certificate of Excellence in Reviewing from Scripta Materialia for 2016, Mar 2017

Dr. Michael Herbig was honoured with the AIME Champion H. Mathewson Award 2017 by the Minerals, Metals & Materials Society (TMS), Jan 2017

Dr. Michael Herbig received the Outstanding Reviewer Award by Acta/Scripta Materialia, 2017

Shyam Katnagallu and Zirong Peng have been awarded with the IFES Student Award of the International Field Emission Society, Aug 2017

Dr. Christoph Kirchlechner has received the Heinz Maier-Leibnitz Preis 2017 (DFG), Berlin (Germany), May 2017

H. Knoll, S. Ocylok, A. Weisheit, H. Springer, E. Jäggle and D. Raabe have been selected for the “Best of Steel 2017” for the article “Combinatorial Alloy Design by Laser Additive Manufacturing”, May 2017

Dr. Fritz Körmann received the VIDI-Preis of the Dutch Science Foundation (NWO) for „Advancing finite-temperature ab initio techniques to explore chemically complex multi-component alloys“, Jul 2017

Dipl.-Ing. Philipp Kürnsteiner won the M&M (Microscopy & Microanalysis) Student Paper Award 2017 with his paper “In-process Precipitation During Laser Additive Manufacturing Investigated by Atom Probe Tomography”. The Prize is annually awarded by the Microanalysis Society, Aug 2017

Xiaolin Li received an “Editor Choice Award 2016” from the Journal of Phase Equilibria and Diffusion, Feb 2017

Chuanlai Liu has been awarded with the Best Oral Presentation Award at the EUROMAT 2017 in Thessaloniki (Greece), Sep 2017

Wei Luo was awarded with the “Best Student Talk Award” at the Nanobrücken 2017 conference in Manchester (UK), Apr 2017

Max-Planck-Institut für Eisenforschung GmbH reaches the 3rd best position in the Humboldt-Ranking among all non-university research organizations in Germany with 30 won scholarships between 2012 and 2016, Sep 2017

Claudia Merola received the Best Poster Award at the 64th American Vacuum Society conference in Tampa, FL (USA), Nov 2017

Enrico Pizzutilo participated in the 67th Lindau Nobel Laureate Meeting, Lake Constance (Germany), Jun 2017

Prof. Dierk Raabe is Vice Chair of the Gordon Research Conference on Physical Metallurgy held at the University of New England in Biddeford, Maine (USA), Jul 2017

Prof. Dierk Raabe is Senator of Helmholtz Society since 2017

Dr. Martin Rabe got a Marie Skłodowska-Curie European Fellowship “Smart cc - Designing novel smart sensor interfaces based on a biologically abundant peptide motif: coiled-coils”, Jun 2017 to May 2019

Dr. Michael Rohwerder received the Excellent Poster Award for the poster entitled: “Novel Zinc-Nanocomposite Coatings for Intelligent Corrosion Protection” at the 11th International Conference on Zinc and Zinc Alloy Coated Steel Sheet (Galvatech 2017) in Tokyo (Japan), Nov 2017

Dr. Rafael Soler was awarded with the Best Poster Award at the ECI Conference (Engineering Conference International) on Small Scale Mechanics, Dubrovnik (Croatia), Oct 2017

Dr. Aleksandar R. Zeradjanin received a Travel Award for Young Electrochemists, in recognition of the quality of scientific research and contribution to the 68th ISE (International Society of Electrochemistry) Annual Meeting, Providence (USA), Aug 2017

2018

Lamy Abdellaoui won the Best Oral Communication Award at the “1st International Meeting on Alternative and Green Energies” (IMAGE18) in Mohammedia (Morocco), May 2018

Prof. Gerhard Dehm received an ERC Advanced Grant for the project “GB-CORRELATE - Correlating the State and Properties of Grain Boundaries”, Mar 2018

Dr. Poulumi Dey received one of two Best Poster Awards at the 3rd International Conference on Metals and Hydrogen „SteelyHydrogen2018” in Ghent (Belgium), May 2018

Aniruddha Dutta won the German Science Slam Championship 2018. In the final eight researchers competed against each other, Wiesbaden (Germany), Nov 2018

Dr. Eric A. Jäggle visited the Tokyo Institute of Technology, Tokyo (Japan), Department of Materials Science and Engineering as specially Appointed Assistant Professor, Mar 2018 to Feb 2020

Dr. Baptiste Gault received an ERC Consolidator Grant for the project „SHINE - Seeing Hydrogen in Matter“, Feb 2018

Dr. Simon Geiger was awarded the prize of the German Chemical Society (GDCh) for his dissertation titled “Stability investigations of iridium-based catalysts towards acidic water splitting”, Aug 2018



Daniel Göhl received a DAAD Fellowship for a research short-term stay at Yuriy Román's Group, Massachusetts Institute of Technology (USA), Sep 2018 to Dec 2018

Ankit Gupta won one of two 2018 Travel Awards sponsored by the journal "Materials" for his paper on "First-principles investigation of thermodynamics and precipitation kinetics in Al-Sc alloys". Ankit Gupta presented his work at the "TMS 2018 Annual Meeting and Exhibition, Phoenix (USA), Mar 2018

Dr. Tilmann Hickel received the Acta Journals Outstanding Review Award for 2017, Apr 2018

Dr. Stefan Hieke was awarded with a EMS (European Microscopy Society) Scholarship 2018 to present his work at the 19th International Microscopy Congress (IMC19) in Sydney (Australia), Sep 2018

Dr. Stefan Hieke was one of 50 selected participants of the Young Scientist Assembly of the International Federation of Societies for Microscopy held before the 19th International Microscopy Congress (IMC19) in Sydney (Australia), Sep 2018

Dr. Reza Darvishi Kamachali was awarded the Heisenberg Fellowship by the German Research Foundation to pursue his research on materials microstructures, Jan 2018

Dr. Christoph Kirchlechner was awarded with the Certificate of Excellence in Reviewing by Acta Materialia and Scripta Materialia, Apr 2018

Philipp Kürnsteiner received the Acta Materialia Student Award 2017 for the best publication of the previous year for the paper "Massive nanoprecipitation in an Fe-19Ni-xAl maraging steel triggered by the intrinsic heat treatment during laser metal deposition", Aug 2018

Dr. Marc Ledendecker received a DAAD Fellowship for a research short-term stay at Alivisatos Group, University of California, Berkeley (USA), Jun to Sep 2018

Dr. Christian Liebscher's paper on "Strain-Induced Asymmetric Line Segregation at Faceted Si Grain Boundaries" was selected as cover story in Physical Review Letters 121(1), Jul 2018

Maisam Merali won the 2018 European Placement Prize of the University of Cambridge for his work on phase relations in the Co-Ti system, which he performed during his two-month summer internship in the group Intermetallic Materials of the SN department, Nov 2018

Prof. Dierk Raabe has been honoured with The Seidmann Family Lecture Series Award, Tel Aviv University (Israel), 2018

Prof. Dierk Raabe and Dr. Michael Herbig and their co-authors have been awarded with the AIME Champion H. Mathewson Award 2018 by The Minerals, Metals & Materials Society (TMS) for their Publication "Autonomous Filling of Grain-Boundary Cavities during Creep Loading in Fe-Mo Alloys". (Zhang, S., Fang, H., Gramsma, M.E. et al. Metall and Mat Trans A (2016) 47: 4831. <https://doi.org/10.1007/s11661-016-3642-0>), Jan 2018

Prof. Christina Scheu was nominated to serve as panel member of the strategic evaluation of the research field Matter of the Helmholtz Association, 2018

Prof. Christina Scheu has been elected as a member of the evaluation board for the "EFRE.NRW 2014–2020 „NeueWerkstoffe.NRW" (European Regional Development Fund of the State of North Rhine-Westphalia), 2018

Dr. Cidem Toparli won an ISE Prize "Oronzio and Niccolò De Nora Foundation Young Author Prize" for her paper "In situ and operando observation of surface oxides during oxygen evolution reaction on copper" in Electrochim. Acta 236 (2017) 104, Aug 2018



Participation in Research Programmes

National:

BMBF

„ECCO2 - Combinatorial electrocatalytic CO2 reduction“, BMBF „Technologies for Sustainability and Climate Protection“, Oct 2011 - Sep 2016

„KoWUB - Novel corrosion protection coatings compatible with hot forming“, BMBF, May 2012 – May 2015

„MANGANESE - Mechanistic investigations of model and applied electrodes for the oxygen evolution“, BMBF, May 2015 – Oct 2019

„NanoSolar - Semiconducting nanocomposites with tailored optical and electronic properties“, BMBF Nano-MatFutur, Jan 2014 – Dec 2019

„Optimizing solar cell efficiency based on 3-dimensinal chemical analysis on the atomistic scale (Optimierung des Wirkungsgrades von Solarzellen basierend auf 3-dimensionalen chemischen Analysen auf atomarer Skala)“, BMBF NanoMatFutur, Feb 2013 – Aug 2015

„RADIKAL - Resource-saving material substitution by additive & intelligent FeAl material concepts adapted for light and functional building“, BMBF MatRessource, Feb 2013 – Mar 2016

„RAVE-K - Ressource friendly design for precious metal containing switch materials for low voltage applications“, BMBF MatRessource, Jun 2013 – May 2016

„UGSLIT - Ultra-high-strength, weight-reduced steels for resource-saving lightweight construction in transport applications“, BMBF, Aug 2016 – Mar 2018

„White Etching Crack - Knowledge-based design of wear resistant bearing steels by atomic-scale characterization as countermeasure against white-etching crack failure in wind power plants“, BMBF, Sep 2016 – Aug 2021

BMW i

„Development of HTPEM fuel cells with improved degradation behaviour via detailed structure and chemical analysis“, BMW i, AiF Projekt GmbH, Jan 2015 – Nov 2017

„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“, BMW i, Apr 2016 – Mar 2019

DFG

DFG Priority Programmes, Collaborative Research Centres & Transregio Projects

„Broadband reflecting fibers with tailored structures inspired by desert ants“, DFG SPP 1839: Tailored Disorder - A science- and engineering-based approach to materials design for advanced photonic applications, Jul 2015 – Dec 2018

„Correlative study towards experimental validation of the high throughput methodology (S02)“, DFG SFB 1232: From colored states to evolutionary structural materials, Jul 2016 – Jun 2020

„Coupling phenomena in magnetocaloric materials: From thin layers to composites“, DFG SPP 1599: Caloric Effects in Ferroic Materials: New Concepts for Cooling, Sep 2012 – Dec 2018

„Electro-plasticity in Al-Cu eutectic alloys“, DFG SPP 1959: Manipulation of matter controlled by electric and magnetic fields: Towards novel synthesis and processing routes of inorganic materials, Jul 2016 – Dec 2019

„Evolution of strengthening phases under in-service stresses and temperatures: phase-field and experimental study“, DFG SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Jul 2017 – Dec 2019



„Investigation and enhancement on bonding by cold bulk metal forming processes“, DFG SPP 1640: Joining by Plastic Deformation, Nov 2011 – Dec 2018

„Investigations of the local alloy composition by means of atom probe tomography (A04)“, DFG CRC/Trans-regios, TRR 103: From Atoms to Turbine Blades - A Scientific Approach for Developing the Next Generation of Single Crystal Superalloys, Jan 2012 – Dec 2019

„Mechano-chemical coupling during precipitate formation in Al-based alloys“, DFG SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Jul 2015 – Apr 2019

„Metallic nanowires on the atomic scale: Electronic and vibrational coupling in real world systems“, DFG Forschungsgruppe 1700, Jul 2016 – Dec 2019

„Metal oxide nanostructures for electrochemical and photoelectrochemical water splitting“, DFG SPP 1613: Fuels Produced Regeneratively Through Light-Driven Water Splitting: Clarification of the Elemental Processes Involved and Prospects for Implementation in Technological Concepts, Jan 2017 – Mar 2019

„Micromechanisms of the electro-plastic effect in magnesium alloys investigated by means of electron microscopy“, DFG SPP 1959: Manipulation of matter controlled by electric and magnetic fields: Towards novel synthesis and processing routes of inorganic materials, Jul 2016 – Dec 2019

„Modeling bainitic transformations during press hardening“, DFG SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical, Jan 2015 – Dec 2016

„PaCCman - Particle-strengthened Compositionally Complex Alloys - interlinking powder synthesis, additive manufacturing, microstructure evolution and deformation mechanisms“, DFG SPP 2006: Compositionally Complex Alloys - High Entropy Alloys (CCA - HEA), Jul 2017 – Dec 2020

„Phase-field-based chemomechanical models for phase transitions and dislocation-microstructure interaction in metallic alloys with application to kappa-carbides“, DFG SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Jun 2017 – Dec 2019

„Quantum mechanically guided design of ultra-strong and damage-tolerant glasses“, DFG SPP 1594: Topological Engineering of Ultra-Strong Glasses, Dec 2015 – Oct 2019

„Steel - *Ab Initio*. Quantum Mechanics Guided Design of New Fe-based Materials“, DFG SFB 761, 1st period: July 2007 – June 2011, 2nd period: Jul 2011 – Jun 2015, 3rd period: Jul 2015 – Jun 2019

Projects at MPIE in frame of SFB 761:

- A 02 *Ab initio* thermodynamics und kinetics in the Fe-Mn-Al-C system, Jul 2007 – Jun 2019
- A 07 Microstructure mechanics and fundamentals of concurrent twinning and martensite formation, Jul 2007 – Jun 2019
- A 09 *Ab initio* based mesoscale simulation of hydrogen embrittlement, Jul 2011 – Jun 2019
- C 01 Microstructure analytics, Jul 2015 – Jun 2019
- C 04 Fatigue, damage and stress corrosion cracking under cyclic loading, Jul 2007 – Jun 2019
- C 08 3D atomic analysis of the local chemical composition by atom probe tomography, Jul 2011 – Jun 2019
- C 10 Deformation behavior of multi-phase steels, Jul 2015 – Jun 2019
- T 4 Influence of microstructure on hydrogen embrittlement in Cr-alloyed high-Mn steels, Jul 2015 – Dec 2018

„Synthetic dental composite materials inspired by the hierarchical organization of shark tooth enameloid“, DFG SPP 1420: Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials, Aug 2013 – Dec 2016

„Tailored precipitation (B₂, L₂) strengthened, compositionally complex FeAlCr (Mn, Co, Ni, Ti) alloys for high temperature applications“, DFG SPP 2006: Compositionally Complex Alloys - High Entropy Alloys (CCA - HEA), Jan 2018 – Dec 2020

„Thermo-chemo-mechanical coupling during thermomechanical processing of microalloyed steels“, DFG SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Jun 2014 – Dec 2017



„Towards self-healing metals by employing optimally-dispersed Ti-Ni shape memory nano-particles“, DFG SPP 1568: Design and Generic Principles of Self-Healing Materials, Apr 2014 – Dec 2017

„TRIP-iCCAs - Interstitial transformation-induced plasticity-assisted quinary compositionally complex alloys: Design, structure and mechanical behavior“, DFG SPP 2006: Compositionally Complex Alloys - High Entropy Alloys (CCA - HEA), Jul 2017 – Dec 2020

„Understanding the damage initiation at microstructural scale (B03)“, DFG CRC/Transregios, TRR 188: Damage Controlled Forming Processes, Feb 2017 – Dec 2020

„Understanding the role of trigger signal spreading, release rate of suitable active agents and their transport rate for optimal healing in extrinsic self-healing materials“, DFG SPP 1568: Design and Generic Principles of Self-Healing Materials, May 2014 – Jun 2018

DFG Research Grants

„Ab initio based calculation of the stability of selected TCP precipitates in steels: Temperature and interface effects“, DFG Research Grant, Feb 2017 – Jan 2020

„AHEAD - Analysis of the Stability of High Entropy Alloys by Dewetting of Thin Films“, DFG-ANR, Mar 2017 – Jul 2020

„Automated analysis and validation of interatomic potentials for application in Materials Science“, DFG Research Grant, Jan 2019 – Dec 2021

„Can high strength and moderate ductility be combined in wear resistant coatings? A fundamental plasticity study of X_2BC nanolaminates ($X=Hf, Mo$)“, DFG Research Grant, Oct 2016 – Dec 2019

„Consistent physically-based modeling of dynamic recrystallization under hot working conditions“, DFG Research Grant, Apr 2016 – Apr 2019

„Correlation of growth, structure, optical and electronic properties of novel $Nb_3O_7(OH)$ and Nb_2O_5 nanostructures“, DFG Research Grant, Jul 2017 – Jun 2020

„CORRKEST - Correlative characterization of co-evaporated $Cu_2ZnSnSe_4$ thin-films“, DFG Research Grant, Apr 2016 – Dec 2019

„Diffusion in high entropy alloys: Development and application of an experiment-ab initio approach“, DFG Research Grant, Jan 2019 – Dec 2021

„Exploring Multinary Nanoparticles by Combinatorial Sputtering into Ionic Liquids and Advanced Transmission Electron Microscopy“, DFG Research Grant, Dec 2016 – Dec 2019

„Fracture initiation in FCC and BCC metals during tribology“, DFG Research Grant, Oct 2017 – Sep 2020

„From interatomic potentials to phase diagrams: Integrated tools for validation and fitting“, DFG Research Grant, Jan 2019 – Dec 2021

„Fundamentals of molecular adhesion for the prediction of macroscopic adhesion at electrified interfaces“, DFG Research Grant, Dec 2015 – Dec 2018

„Hydrogen-microstructure interactions in iron-based alloys at small scales: from amorphous, via nanocrystals, to polycrystals“, DFG Research Grant, Sep 2016 – Aug 2018

„Lamellar Fe-Al in situ composite materials: microstructure and mechanical properties“, DFG Research Grant, Jan 2013 – Aug 2016

„Magnetism in iron alloys: thermodynamics, kinetics and defects“, DFG-ANR, Feb 2017 – Jan 2020

„Materials World Network: Fundamentals of Peptide Materials - Experimental and Simulation Probes“, DFG-NSF, Sep 2013 – Nov 2016

„Precipitation kinetics during non-linear heat treatment in Laser Additive Manufacturing“, DFG Research Grant, Jun 2016 – Apr 2019

„Rare-earth based alloys for hard-magnetic applications: Temperature and pressure dependent phase stabilities“, DFG-ANR, Jan 2017 – Jun 2020

„Structure, phase formation and properties of metallic glasses manipulated by electric current“, DFG Research Grant, May 2017 – Dec 2020



„Study of grain-boundary-dislocation interactions by advanced in situ μ Laue diffraction“, DFG Research Grant, Jan 2015 – Jan 2019

„The effective pH at the solid-liquid interface and the local ion distribution during complex electrochemical reactions“, DFG Research Grant, Mar 2014 – Mar 2017

„Understanding the role of dislocation distribution(s) on the slip transfer across twin-boundaries“, DFG Research Grant, Aug 2015 - Dec 2018

„xMicroFatigue - X-ray Laue Microscopy to Understand Fatigue Damage“, DFG-ANR, Feb 2017 – Feb 2020

DFG Cluster of Excellence

„Electrochemistry on „dry surfaces“: electrode potential and structural order in nanoscopic electrolyte layers“, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Aug 2013 – Dec 2018

„Probing the molecular structure of extended solvated surfaces and interfaces“, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Mar 2014 – Feb 2017

„Stability of electrode materials in an electrochemical environment“, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Mar 2016 – Feb 2019

„Zinc oxide – water interfaces: interaction-driven structural evolution“, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Feb 2015 – Jul 2016

Max Planck Society

„AProLAM - Advanced Alloy and Process Design for laser Additive Manufacturing of Metals“, MPG - FhG cooperation, Apr 2015 – Dec 2018

„Combinatorial design of novel rare-earth free, high-entropy based permanent magnets“, Indian Institute of Technology, Madras, Max Planck Partner Group with India, Jun 2018 – May 2021

„Initial wear - Early detection of material wear in high-precision machine tools“, MPG - FhG cooperation, Jan 2014 – Dec 2016

„International Max Planck Research School for Interface Controlled Materials for Energy Conversion IMPRS-SurMat (IMPRS - SurMat)“, Max Planck Society, Jan 2016 – Dec 2021

„Designing Damage Tolerant Functional Oxide Nanostructures: Damage Tolerance Studies on Barium Titanate at Small Length Scales“, Indian Institute of Technology Bombay, Max Planck Partner Group with India, Mar 2017 – Mar 2020

„MaxNet BigMax - Max Planck Research Network on big-data-driven material science“, Research Cooperation, Max Planck Society, Mar 2017 – Mar 2022

„MaxNet Energy“, Research Cooperation, Max Planck Society, Jan 2014 – Dec 2018

„Stress and defects driven phase transformations“, Indian Institute of Technology, Roorkee, Max Planck Partner Group with India, Apr 2017 – Apr 2020

Leibniz Association

„CarMON - New Carbon-Metal Oxide Nanohybrids for Efficient Energy Storage and Water Desalination“, Leibniz Competition, May 2017 – Apr 2020

Volkswagen Stiftung

„A new class of smart materials: Switching strength for future´s safety“, Experiment!, Jan 2017 – Apr 2018

„Seeing atoms in biological materials“, Experiment!, Jan 2017 – Jun 2018

KSB Stiftung

„Investigation of structural transformations at grain boundaries in Ti and Ti alloys by high-resolution and in-situ transmission electron microscopy“, KSB Stiftung, Jan 2018 – Dec 2018

International:

Christian Doppler Society

Christian Doppler Laboratory „Diffusion and segregation mechanisms during production of high strength steel sheet” (original title: “Diffusions- und Segregationsvorgänge bei der Produktion hochfesten Stahlbands”) Jan 2008 – Dec 2015

FWO - Fonds Wetenschappelijk Onderzoek

„PredictCor - Knowledge and technology platform for prediction of durability and lifetime of organic coated metals under long-term environmental corrosion”, FWO/NL, Jan 2018 – Dec 2021

European Union

European Research Council

„GB-CORRELATE - Correlating the State and Properties of Grain Boundaries“, ERC Advanced Grant, Horizon 2020, Aug 2018 – Jul 2023

„SHINE - Seeing Hydrogen in Matter“, ERC Consolidator Grant, Horizon 2020, Feb 2018 – Jan 2023

„SMARTMET - Adaptive nanostructures in next generation metallic materials: Converting mechanically unstable structures into smart engineering alloys“, ERC Advanced Grant, FP 7, Feb 2012 – Jan 2017

„TIME-BRIDGE - Time-scale bridging potentials for realistic molecular dynamics simulations“, ERC Starting Grant, Horizon 2020, Jul 2015 – Jun 2020

Marie Skłodowska-Curie Actions (FP7 and Horizon 2020)

„EIWBinsTEM - Development of electrochemical water based in-situ TEM and study of platinum based nanoparticles potential- and time-dependent changes“, Marie Curie Intra European Fellowship, FP7, Apr 13 – Mar 2016

„Smartcc - Designing novel smart sensor interfaces based on a biologically abundant peptide motif“, Marie Skłodowska-Curie European Fellowship, Horizon 2020, Jun 2017 – May 2019

„SOMATAI - Soft Matter at Aqueous Interfaces“, Marie Curie Initial Training Network, FP7, Oct 2012 – Mar 2016

Collaborative Projects (FP7 and Horizon 2020)

„AccMet - Accelerated Metallurgy - the accelerated discovery of alloy formulations using combinatorial principles“, Collaborative project, FP7, Jun 2011 – Jun 2016

„EPPL - Enhanced Power Pilot Line“, ENIAC Joint Undertaking, FP7, May 2013 – Sep 2016

„HERCULES-2 - Fuel flexible, near-zero emissions, adaptive performance marine engine“, Horizon 2020 Societal Challenges - Smart, Green And Integrated Transport, May 2015 – Oct 2018

„PowerBase - Enhanced substrates and GaN pilot lines enabling compact power applications“, The ECSEL Joint Undertaking, FP7, May 2015 – Apr 2018

RFCS (Research Fund for Coal and Steel)

„JOINOX - Guidelines for use of welded stainless steel in corrosive environments“, RFCS, Sep 2012 – Feb 2016

„LIGHTTOUGH - Screening of tough lightweight Fe-Mn-Al-C steels using high throughput methodologies“, RFCS, Jul 2015 – Dec 2018

„MicroCorr - Improving steel product durability through alloy coating microstructure“, RFCS, Sep 2015 – Feb 2019



„MuSTMef - Multi Scale Simulation Techniques for Metal Forming“, RFCS, Jul 2016 – Jun 2020

„OPTIBOS - New developments and optimisation of high strength boron treated steels through the application of advanced boron onitoring techniques“, RFCS, Jul 2012 – Dec 2015

„TOOLMART - New Metallurgical Tools for optimum design of modern Ultra High Strength Low Carbon Martensitic Steels“, RFCS, Jul 2013 – Dec 2016

European Space Agency (ESA)

„On Beryllium Alloy & Composite Development for Space and Non-Space Application“, Jan 2014 – Dec 2016

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), Aug 2018 – Dec 2022



Collaboration with National and International Research Institutes

National:

Brandenburgische Technische Universität Cottbus-Senftenberg: Lehrstuhl Konstruktion und Fertigung (KuF), Cottbus

Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin

Deutsche Akademie der Naturforscher Leopoldina, Halle

Deutsches Zentrum für Luft- und Raumfahrt (DLR), Bonn

Forschungszentrum Jülich GmbH, Jülich

Forschungszentrum Jülich GmbH: Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen (ER-C), Jülich

Forschungszentrum Jülich GmbH: Institute of Complex Systems Soft Condensed Matter (ICS-3), Jülich

Forschungszentrum Jülich GmbH: Institut für Energie- und Klimaforschung, Werkstoffstruktur und -eigenschaften (IEK-2), Jülich

Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V., München

Fraunhofer Institut für Lasertechnik (ILT), Aachen

Fraunhofer Institut für Produktionstechnologie (IPT), Aachen

Fraunhofer Institut für Werkstoffmechanik (IWM), Freiburg

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

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

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für allgemeine Werkstoffeigenschaften, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Feststoff- und Grenzflächen-verfahrenstechnik, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Korrosion und Oberflächentechnik, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Kunststofftechnik, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Werkstoffkunde und Technologie der Metalle, Erlangen

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

Heinrich-Heine-Universität Düsseldorf: Institut für Experimentelle Physik der kondensierten Materie, Düsseldorf

Heinrich-Heine-Universität Düsseldorf: Institut für Medizinische Mikrobiologie und Krankenhaushygiene, Düsseldorf

Heinrich-Heine-Universität Düsseldorf: Institut für Theoretische Physik, Düsseldorf

Heinrich-Heine-Universität Düsseldorf: Lehrstuhl für anorganische Chemie, Düsseldorf

Heinrich-Heine-Universität Düsseldorf: Lehrstuhl für organische Chemie, Düsseldorf

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

Helmholtz-Zentrum Berlin, Berlin

Helmholtz-Zentrum-Berlin für Materialien und Energie, Berlin

Helmholtz-Zentrum Geesthacht, Zentrum für Material- und Küstenforschung, Mg Innovation Center (MagIC), Geesthacht



Humboldt Universität zu Berlin: Institut für Mathematik, Berlin
IFW Dresden, Institute for Complex Materials, Dresden
Karlsruher Institut für Technologie (KIT): Institut für Angewandte Materialien – Werkstoffkunde (IAM), Karlsruhe
Karlsruher Institut für Technologie (KIT): Institut für Technikfolgenabschätzung und Systemanalyse, Karlsruhe
Karlsruher Institut für Technologie (KIT): Institut für thermische Strömungsmaschinen, Karlsruhe
Leibniz-Institut für Analytische Wissenschaften e.V. (ISAS), Dortmund
Leibniz-Institut für Festkörper- und Werkstoffforschung(IFW): Institut für komplexe Materialien, Dresden
Leibniz-Institut für Neue Materialien (INM), Saarbrücken
Leibniz-Institut für Plasmaforschung und Technologie (INP), Greifswald
Leibniz-Institut für Werkstofforientierte Technologien (IWT), Bremen
Leibniz Universität Hannover: Institut für Festkörperphysik, Hannover
Leibniz Universität Hannover: Institut für Werkstoffkunde, Hannover
Ludwig-Maximilians-Universität (LMU): Fakultät für Chemie und Pharmazie, München
Max-Planck-Institut für Chemische Energiekonversion, Mülheim a. d. Ruhr
Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden
Max-Planck-Institut für Festkörperforschung, Stuttgart
Max-Planck-Institut für Innovation und Wettbewerb, München
Max-Planck-Institut für Intelligente Systeme, Stuttgart
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Collaborating Industrial Partners and Patents

Collaborating Industrial Partners

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Patents

Patents issued in the given time schedule

Date of Issue	Description	Inventors
June 07, 2018	Fabrication of nanoporous carbide membranes Joint invention with Universitat Politècnica de Catalunya (EP 2 664 683)	Renner, Frank, Dr. Duarte-Correa, Maria Jazmin, Dr. Lengsfeld, Julia Bruna, Pere, Dr., BarcelonaTech
utility patent August 18, 2016	Multi purpose method cell (20 2016 104 543.6)	Kerger, Philip Rohwerder, Michael, Dr.
March 03, 2016	Nanoelektroden-Partikelfalle für empfindliche spektroskopische und elektronische Analyse Joint invention with Academia Sinica Taipei (TWI490487)	Erbe, Andreas, Dr. Chu, Chia-Fu, PhD, Academia Sinica Taipei Chu, Ming-Li, PhD, Academia Sinica Taipei Lesser-Rojas, Leonardo, Academia Sinica Taipei

Patents filed in the given time schedule

Date of Pending	Description	Inventors
January 20, 2016	Flat steel product and method for the production thereof Joint invention with ThyssenKrupp Steel Europe AG (PCT/EP2016/051109)	Palm, Martin, Dr. Ponge, Dirk, Dr. Leitner, Andreas Hofmann, Harald, Dipl.-Ing., ThyssenKrupp Steel Europe Schirmer, Matthias, Dipl.-Ing. ThyssenKrupp Steel Europe Grövert, Michael, ThyssenKrupp Steel Europe Ferkel, Hans, Prof. Dr., ThyssenKrupp Steel Europe
August 31, 2016	Hochduktile Mg-Al-Ca-Legierung (10 2016 116 244.2)	Neugebauer, Jörg, Prof. Raabe, Dierk, Prof. Sandlöbes, Stefanie, Dr. Friak, Martin, Dr. Pei, Zongrei, Dr.
October 25, 2016	Process for recycling of noble metals (PCT/ DE2016/ 100498)	Mayrhofer, Karl, Dr. Hodnik, Nejc, Dr. Baldizzone, Claudio, Dr.



Date of Pending	Description	Inventors
February 02, 2018	Hydroxylapatit Joint invention with Dr. Kurt Wolff GmbH & Co. KG (10 2018 102 365.0)	Fabritius, Helge, Dr. Enax, Joachim, Dr., Firma Wolff Klenk, Adolf, Dr., Firma Wolff
September 2018	Heizung für Mikro- Verformungseinrichtung (18199374.2)	Argela, Viswanath Gowtham Kirchlechner, Christoph, Dr. Gonzalez, Iwan Kölling, Michael



Conferences, Symposia and Meetings Organized by the Institute

2015 (not included in the Scientific Report 2013 - 2015)

A. Erbe, C. Arckel and C.D. Fernández-Solis organized the training course “Career Development” for fellows of the Marie Curie Initial Training Network “SOMATAI” at the MPIE, Düsseldorf (Germany), Dec 2015

M. Palm co-organized and chaired the session “Frontiers in Intermetallics” within the framework of the international conference „Advances in Materials & Processing Technologies - AMPT 2015“ in Madrid (Spain), Dec 2015

2016

G. Dehm, C. Scheu, and S. Brinckmann organized the “Mechanics meets Energy IV” symposium at Akademie Biggese in Attendorn (Germany), 18 - 21 Jan 2016

G. Dehm co-organized the Symposium “In situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science” at DPG Spring Meeting 2016 in Regensburg (Germany), 06 - 11 Mar 2016

J. Neugebauer co-organized the Topical Session “Integrated computational materials engineering for design of new materials” at the Spring Meeting of the German Physical Society (DPG) in Regensburg (Germany), 06 - 11 Mar 2016

M. Palm and F. Stein together with F. Pyczak (Helmholtz-Zentrum Geesthacht) co-organized and co-chaired the priority topic “Hochtemperaturwerkstoffe” (high temperature materials) at the 62. Metallkunde Kolloquium in Lech am Arlberg (Austria), Apr 2016

F. Archie organized the 26th GLADD Meeting held at the MPIE, Düsseldorf (Germany), 16 Apr 2016

F. Roters co-organized the Mini-Symposium “Fourier-based Methods for Computing the Behavior of Heterogeneous Materials Developments, Extensions and Applications” during the European Congress on Computational Methods in Applied Sciences and Engineering ECCOMAS 2016 in Kreta (Greece), 05 - 10 May 2016

B. Gault was Co-Chair at the Biannual „NRW-APT User Meeting“ at the MPIE, Düsseldorf (Germany), 18 May 2016 and 15 Nov 2016

M. Todorova co-organized the 2nd German-Dutch Workshop on “Computational Materials Science” in Domburg (The Netherlands), 26 - 29 Jun 2016

E. A. Jäggle organized the event “Alloys for Additive Manufacturing Workshop 2016” held at the MPIE in Düsseldorf (Germany) with 80 participants, 04 - 05 Jul 2016

F. Roters organized the 5th International Symposium on “Computational Mechanics of Polycrystals, CMCn 2016” and the “1st DAMASK User Meeting” held at the MPIE, Düsseldorf (Germany), 01 - 02 Sep 2016

S. Brinckmann co-organized the symposium „Tribology across length-scales: Experiments and simulations“ at the Materials Science Engineering in Darmstadt (Germany), 27 - 29 Sep 2016

M. Rohwerder organized the Symposium C06 “Metallic, Organic and Composite Coatings for Corrosion Protection” at the 230th Meeting of the Electrochemical Society - PRiME2016 in Hawaii (USA), Oct 2016

T. Hickel and J. Neugebauer organized the ADIS 2016 Workshop “Ab initio Description of Iron and Steel: Mechanical properties” at Ringberg Castle, Kreuth (Germany), 03 - 07 Oct 2016

J. Neugebauer co-organized the Symposium „Materials design: where condensed-matter physics and big-data informatics meet” at the MMM 2016 Conference in Dijon (France), 09 - 14 Oct 2016

F. Roters co-organized the Symposium “Microstructure evolution in materials: mechanisms, properties, manufacture” during the 8th International Conference on Multiscale Materials Modeling, Dijon (France), 09 - 14 Oct 2016



J. Neugebauer co-organized the Symposium “Design, Discovery, and Understanding of Materials Guided by Theory, Computation and Data Mining” at the MRS Fall Meeting 2016 in Boston (USA), 27 Nov - 02 Dec 2016

K. Hübel, M. Rohwerder, C. Scheu and M. Todorova organized the workshop “Status and Future Challenges in Characterisation of Interfaces for Electrochemical Applications - Part 1” at the MPIE, Düsseldorf (Germany), 05 Dec 2016

2017

G. Dehm, C. Scheu, and S. Brinckmann organized the “Mechanics meets Energy V” symposium at Ringberg Castle, Kreuth (Germany), 08 - 12 Jan 2017

C. Scheu organized the “Hydrogen Technology” Meeting at the MPIE, Düsseldorf (Germany), 25 Jan 2017

T. Hickel co-organized the Symposium “Advanced High-Strength Steels” at the TMS Meeting in San Diego (USA), 26 Feb - 2 Mar 2017

J. Neugebauer co-organized the Topical Session “Data driven materials design” at the Spring Meeting of the German Physical Society (DPG) in Dresden, 19 - 24 Mar 2017

B. Gault was Co-Chair at the “International workshop: high electric fields in electrochemistry and in atom probe tomography” at Ringberg Castle, Kreuth (Germany), 29 Mar - 1 Apr 2017

M. Todorova, J. Neugebauer, S. Wippermann and G. Gault organized the Workshop “High electric fields in electrochemistry and in atom probe tomography” at Ringberg Castle, Kreuth (Germany), 29 Mar - 1 Apr 2017

S. Brinckmann co-organized the „Frontiers in Material Science & Engineering: Hydrogen Interaction in Metals“ Workshop at the MPIE, 11 Apr 2017

G. Dehm co-organized the topic day “Lokale Charakterisierungsmethoden in der Werkstoffforschung“ at the Metallkundekolloquium/Arlbergkolloquium in Lech (Austria), 19 - 21 Apr 2017

G. Dehm co-organized the symposium “Mechanical Properties and Adhesion” at the 44th ICMCTF (International Conference on Metallurgical Coatings and Thin Films) in San Diego (USA), 24 - 28 April 2017

T. Hickel organized the “Fe-X French-German discussion meeting” at the MPIE, Düsseldorf (Germany), 15 - 16 May 2017

K. Hübel, K. Mayrhofer, M. Rohwerder, C. Scheu and M. Todorova organized the workshop “Status and Future Challenges in Characterisation of Interfaces for Electrochemical Applications - Part 2” at the MPIE, Düsseldorf (Germany), 16 Aug 2017

G. Dehm co-organized the symposium “Environmental, in-situ and time-resolved microscopy” at MC 2017 (Microscopy Conference 2017) in Lausanne (Switzerland), 21 - 25 Aug 2017

S. Zaeferrer and T. Griffiths organized and chaired the workshop “3D Materials characterization on all length scales and its applications to iron and steel” held at the MPIE in Düsseldorf (Germany) with 75 participants, 29 Aug 2017

M. Todorova co-organized the CM - ICAMS Workshop in Eberburg (Germany), 04 - 07 Sep 2017

B. Gault was Symposium Chair at the special symposium for the 50th Anniversary of the “Atom Probe, Microscopy & Microanalysis 2017” in Saint Louis (USA), 06 - 10 Sep 2017

E. A. Jäggle co-organized the conference “Alloys for Additive Manufacturing Symposium 2017” with 120 participants, held at EMPA, in Dübendorf (Switzerland), 11 - 12 Sep 2017

C. Kirchlechner co-organized the “Summer School on Experimental Nano- and Micromechanics” at the MPIE, Düsseldorf (Germany), 11 - 15 Sep 2017

M. Rohwerder co-organized the Symposium C04 “Coatings and Inhibitors” at the 232nd Meeting of the Electrochemical Society in National Harbor (USA), Oct 2017

M. Palm and F. Stein co-organized the international conference “Intermetallics 2017” at the Educational Center Kloster Banz, Bad Staffelstein (Germany), 02 - 06 Oct 2017



C. Scheu organized the “100 year MPIE Anniversary Colloquium” at the MPIE, Düsseldorf (Germany), 5 Oct 2017

B. Gault was Co-Chair at the Biannual „NRW-APT User Meeting“ at the MPIE, Düsseldorf (Germany), 16 May 2017 and 23 Nov 2017

2018

D. Raabe chaired and *E. A. Jäggle* coordinated the work group “Additive Manufacturing and 3D printing” of the National Academy of Sciences Leopoldina, 2018

J. Janßen and *J. Neugebauer* organized a 1st Piron-Workshop at the MPIE, Düsseldorf (Germany), 09 Jan 2018

M. Todorova co-organized the 3rd Austrian-German Workshop “Computational Materials Science on Complex Energy Landscapes” in Kirchdorf (Austria), 15 - 19 Jan 2018

G. Dehm co-organized the symposium “Fundamentals of mechanical response” at the “Conference on Electronic and Advanced Materials” in Orlando (USA), 17 - 19 Jan 2018

C. Scheu co-organized the symposium “Experimental and Theoretical insights on Interfaces of Ceramics” at the “Conference on Electronic and Advanced Materials” in Orlando (USA), 17 - 19 Jan 2018

G. Dehm, *C. Scheu*, and *S. Brinckmann* organized the “Mechanics meets Energy VI” symposium at Kloster Steinfeld, Kall (Germany), 29 Jan - 2 Feb 2018

G. Dehm co-organized the topic day “Dislocation based plasticity - experiment vs. simulation” at “The Schöntal Symposium Dislocation-based Plasticity” of the DFG Forschergruppe FOR 1650 in Schöntal (Germany), 25 Feb - 02 Mar 2018

T. Hickel co-organized the Symposium “Advanced High-strength Steels” at the TMS 2018 Annual Meeting & Exhibition in Phoenix (USA), 11-15 Mar 2018

G. Dehm co-organized the topical session “Mechanical Properties at Small Scales” at the DPG-Spring Meeting 2018 in Berlin, 11 - 16 Mar 2018

T. Hickel co-organized the Topical Session “Hydrogen in Materials” at the Spring Meeting of the German Physical Society (DPG) in Berlin (Germany), 11 - 16 Mar 2018

T. Hickel co-organized the Topical Session “Magnetism in Materials Science: Thermodynamics, Kinetics and Defects” at the Spring Meeting of the German Physical Society (DPG) in Berlin (Germany), 11 - 16 Mar 2018

C. Kirchlechner co-organized a session on “Experimental Nanomechanics” at the “16th European Mechanics of Materials Conference” in Nantes (France), 26 - 28 Mar 2018

G. Dehm co-organized the topic day “Novel materials and alloy design - microstructure property relationship” at the Metallkundekolloquium/Arlbergkolloquium in Lech (Austria), 09 - 11 Apr 2018

J. Neugebauer co-organized the “BigMax Workshop 2018” on “Big-Data-Driven Materials Science” in Kloster Irsee (Germany), 10 - 13 Apr 2018

G. Dehm co-organized the symposium “Mechanical Properties and Adhesion 45th ICMCTF” (International Conference on Metallurgical Coatings and Thin Films) in San Diego (USA), 23 - 27 Apr 2018

T. Hickel organized the “Fe-X French-German discussion meeting” at the MPIE, Düsseldorf (Germany) from 15 - 16 May 2017

M. Herbig organized a conference session of Correlative Methods at the Atom Probe Tomography & Microscopy conference in Washington (USA), 10 - 15 Jun 2018

F. Roters co-organized the Mini-Symposium “Computational modeling and experimental investigations of metallic materials across scales” during the 6th European Conference on Computational Mechanics in Glasgow (Scotland), 11 - 15 Jun 2018

G. Dehm co-organized the mini-symposium “Experimental Micromechanics and Nanomechanics” at the “10th edition of the European Solids Mechanics Conference” in Bologna (Italy), 02 - 06 Jul 2018



- G. Dehm* co-organized the Gordon Research Conference “Thin Film and Small Scale Mechanical Behavior” in Lewiston (USA), 15 - 20 Jul 2018
- C. Scheu* co-organized the symposium “PS12 - Materials for Energy Production, Storage and Catalysis” at the “19th International Microscopy Congress” in Sydney (Australia), 09 - 14 Sep 2018
- F. Roters* organized the 6th International Symposium on “Computational Mechanics of Polycrystals, CMCn 2018” and the “2nd DAMASK User Meeting” held at the MPIE, Düsseldorf (Germany), 17 - 19 Sep 2018
- R. Hadian* co-organized the Symposium “Predicting Interface Structure and Dynamics - From Atomic- to Meso-Scale” at the MSE 2018 Congress in Darmstadt, 26 - 28 Sep 2018
- S. Brinckmann* co-organized the symposium „Experiments and Simulations Towards Understanding Tribology Across Length-Scales“ at the Materials Science Engineering in Darmstadt (Germany), 26 - 28 Sep 2018
- E. A. Jäggle* co-organized the symposium “Additive Manufacturing - Composites and Complex Materials” at MS&T conference in Columbus (USA), Oct 2018
- M. Herbig* organized a MPIE Workshop ‘Mechanisms of White Etching Matter Formation’ held at the MPIE, Düsseldorf (Germany), 23 Oct 2018
- M. Kühbach and M. Diehl* organized the symposium “From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing” at the Multiscale Materials Modeling (MMM) conference in Osaka (Japan), 28 Oct - 02 Nov 2018
- T. Hickel* co-organized the Symposium „Data-Driven and Physics-Informed Materials Discovery and Design“ at the 9th Multiscale Materials Modelling Conference (MMM 2018) in Osaka (Japan), 28 Oct - 02 Nov 2018
- T. Hickel and J. Neugebauer* organized the ADIS 2018 Workshop “Ab initio Description of Iron and Steel: Thermodynamics, Kinetics and Defects” at Ringberg Castle, Kreuth (Germany), 04 - 09 Nov 2018
- G. Dehm, B. Gault, D. Raabe and C. Scheu* organized the “Opening symposium for advanced (S)TEM and APT facilities” at the MPIE, Düsseldorf (Germany), 05 - 06 Nov 2018
- J. Neugebauer, S. Wippermann, E. Gattermann and R. Groever* organized the “Topical Joint Workshop IMPRS-SurMat & IMPRS RECHARGE about Catalysis and Corrosion: Towards an Atomistic Understanding of Reactions at Interfaces” at the MPIE, Düsseldorf (Germany), 20 Nov 2018



Institute Colloquia and Invited Seminar Lectures

2016

S. Biermann, Centre de Physique Theorique, Ecole Polytechnique, France: Spectral Properties of Correlated Electron Materials from First Principles - Where Do We Stand? (07 Jan 2016)

I. Eremin, Institute for Theoretical Physics III, Ruhr-University Bochum, Germany: Superconductivity in Fe-based Superconductors: Competing Orders and Pairing Fluctuations (12 Jan 2016)

O. Glushko, Erich Schmid Institute of Materials Science, Leoben, Austria: Strain-induced Room Temperature Grain Coarsening: Side Effect or Major Energy Dissipation Mechanism? (14 Jan 2016)

G. Hummer, MPI for Biophysics, Frankfurt/Main, Germany: Extracting Accurate Free Energy Surfaces and Rates from Single-Molecule Pulling Experiments (18 Jan 2016, Colloquium)

J. Haubrich, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany: Ti-Interfaces for Aging-resistant Bonding between Metals and Thermoplastics (18 Jan 2016)

T. F. Kelly, Division Vice President for Innovation and New Technologies, CAMECA Instruments, Inc., Madison, WI, USA: Atomic-Scale Tomography: An Achievable Vision (29 Jan 2016)

P. R. Rios, Universidade Federal Fluminense, Rio de Janeiro, Brazil: Grain Boundary, Triple Junction and Quadruple Point Mobility Controlled Normal Grain Growth (01 Feb 2016)

L. Dezerald, Institut Jean Lamour, Université de Lorraine, Nancy, France: Plastic Anisotropy and Dislocation Glide in bcc Metals (03 Feb 2016)

X. Fang, Tsinghua University, Beijing, China: Stress and Diffusion Coupling during Oxidation at High Temperature (16 Feb 2016)

A. Winkelmann, Bruker Nano GmbH, Berlin, Germany: Applications of Dynamical Electron Diffraction Simulations in the SEM (10 Mar 2016)

M. Gouné, Métallurgie et Matériaux Fonctionnels, ICMCB-CNRS, France: New Insights into Alloying Elements Interaction with α -Ferrite/ γ -Austenite Migrating Interface in Fe-C-Mn System (18 Mar 2016)

F. Danoix, Université de Rouen, France: Combined Atom Probe Tomography and Electron Microscopy Investigation of Intermediate Carbides Precipitation from Supersaturated Virgin Fe-Ni-C Martensites (07 Apr 2016)

A. Ektarawong, Department of Physics, Linköping University, Linköping, Sweden: Theoretical Study of Configurational Disorder in Boron Carbide Modeled by the Superatom-Special Quasirandom Structure Approach (11 Apr 2016)

O. Gutfleisch, TU Darmstadt, Germany: Re-thinking Rare Earth Magnets for Energy Applications: Demand, Sustainability and the Reality of Alternatives (12 Apr 2016, Colloquium)

B.W.J. Clegg, University of Cambridge, UK: Softening Non-Metallic Crystals by Inhomogeneous Elasticity (04 May 2016, Colloquium)

A. Deschamps, Frederic De Geuser, Grenoble Institute of Technology, France: Precipitation in Al-Alloys (04 May 2016)

P. A. van Aken, MPI for Solid State Research, Stuttgart, Germany: Structural Defects and Local Interfacial Chemistry of Complex Oxide Heterointerfaces (23 May 2016, Colloquium)

P. Pant, Indian Institute of Technology-Bombay, Mumbai, India: Role of Orientation and Grain Interactions on the Deformation of Ti64 (23 May 2016)

U. Dahmen, National Center for Electron Microscopy, Molecular Foundry, LBNL, Berkeley, CA, USA: Atomic Resolution Observations of Step Structure and Dynamics in Grain Boundaries (24 May 2016, Colloquium)

I. Vrejoiu, Institute of Physics II, University of Cologne, Germany: Driving Forces and Challenges of Interfacial Functional Oxide Perovskites (13 Jun 2016)

S. Ahmadi, University of Erlangen-Nuremberg, Germany: Stochastic KMC-FEM Modelling of Avalanche Phenomena in Creep Deformation of Bulk Metallic Glasses (14 Jun 2016)

K. Lejaeghere, Center for Molecular Modeling, Ghent University, Belgium: Error Overload? Dealing with DFT Uncertainty (14 Jun 2016)

D. Blavette, Normandie University, Rouen, France: Phase Transformations: Atom-Probe Tomography versus Modeling (23 Jun 2016, Colloquium)



- G. Kresse, Faculty of Physics, University of Vienna, Austria: The Relation between RPA and GW - Forces and Singles (05 Jul 2016)
- M. Huang, The University of Hong Kong, China: Deformation Mechanisms of TWIP Steel: From Micro-pillars to Bulk Samples (06 Jul 2016)
- C. C. Fu, DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France: Diffusion Mechanisms of Solutes in α -Iron Systems (08 Jul 2016)
- X. Maeder, Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland: *In Situ* HR-EBSD Characterization during Micromechanical Testing (12 Jul 2016)
- M. Kabel, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik (ITWM), Kaiserslautern, Germany: Composite Voxels for Nonlinear Mechanical Problems (21 Jul 2016)
- S. Singh, MPI for Chemical Physics of Solids, Dresden, Germany: Nature and Origin of Structural Modulation in Ni_2MnGa Magnetic Shape Memory Alloy (19 Jul 2016)
- M. Beetz, Ludwig-Maximilians-University Munich, Germany: Parameter Analysis and Performance Improvement of Discrete Iterative Reconstruction Techniques in Electron Tomography (20 Jul 2016)
- K. Hameyer, RWTH Aachen University, Germany: Magnetic Material Modeling for Numerical Simulation of Electrical Machines (22 Jul 2016)
- M. Zamanzade, Saarland University, Germany: Environmental Effects on the Mechanical Properties of Metals (22 Jul 2016)
- M. Elhebeary, University of Illinois at Urbana-Champaign, IL, USA: A Pull-to-Bend Testing Technique for Testing Single Crystal Silicon (03 Aug 2016)
- G. M. Stocks, Materials Theory Group, Oak Ridge National Laboratory, TN, USA: Tuning Materials Properties through Extreme Chemical Complexity (24 Aug 2016, Colloquium)
- A. Linscheid, Department of Physics, University of Florida, USA: From the Crystal Structure to the Superconducting T_c : The Role of First Principles Calculations in Computing Superconducting Properties of Real Materials (31 Aug 2016)
- L. Mädler, Foundation Institute of Materials Science (IWT), Department of Production Engineering, University of Bremen, Germany: High-Throughput with Particle Technology (05 Sep 2016, Colloquium)
- N. Rolland, Université de Rouen, France: Some New Ideas to Model Artefacts in Atom Probe Tomography: Application to 3D Reconstruction (08 Sep 2016)
- M. Schroeder, Ruhr-University Bochum, Germany: Lattice Dynamics in Hybrid Perovskite MAPbI_3 (29 Sep 2016)
- M. Chandross, Materials Science and Engineering Center, Sandia National Laboratories, Albuquerque, NM, USA: Linking Microstructural Evolution and Tribology in Metallic Contacts (30 Sep 2016)
- I. Baker, Dartmouth College, Hanover, NH, USA: Microstructures and Mechanical Behavior of $\text{FeNiMnAl}(\text{Cr})$ Alloys (06 Oct 2016, Colloquium)
- H.-H. Heyn, Norwegian University of Science and Technology, Trondheim, Norway: Molecular Dynamics Simulation of Nanoindentation of fcc and bcc Systems: Influence of Hydrogen and Vacancies (18 Oct 2016)
- K. Haenen, Hasselt University, Belgium: Doping Induced Properties of Nanocrystalline CVD Diamond Films and Particles (08 Nov 2016, Colloquium)
- C. W. Sinclair, The University of British Columbia, Vancouver, Canada: Predicting Solute Segregation Kinetics and Properties in Binary Alloys from a Dynamical Variational Gaussian Model (09 Nov 2016)
- O. Prymak, Inorganic Chemistry and Center for Nanointegration Duisburg-Essen (CeNIDE), Germany: Investigation of Nanostructural Materials by means of X-Ray Powder Diffraction (16 Nov 2016)
- S. Kölling, Technische Universiteit Eindhoven, The Netherlands: Disassembling Nanostructures Atom by Atom (17 Nov 2016)
- T. Wang, Interdisciplinary Centre For Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany: Calculation of Phonon Scattering and Thermal Conductivity at Atomistic Scale (21 Nov 2016)
- M. Eberhart, Molecular Theory Group, Colorado School of Mines, CO, USA: The Search for Charge Density Based Structure-Property Relationships (07 Dec 2016, Colloquium)
- I. MacLaren, University of Glasgow, Scotland: Quantitative Analysis of Nanoscale Carbonitrides in High-Mn Steel (07 Dec 2016)
- D. G. Sangiovanni, Interdisciplinary Centre For Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany and Department of Physics, Chemistry, and Biology (IFM), Linköping University, Linköping, Sweden: Mass Transport in Solid Crystals: Equilibrium and Accelerated Molecular Dynamics Investigations (07 Dec 2016)



2017

O. Waseda, MATEIS Lab. INSA de Lyon, France: Atomic Scale Investigation of Cottrell Atmospheres in Steel (09 Jan 2017)

Y. Funakawa, Head of the research department for automotive steel, JFE Steel Corporation, Chiyoda, Tokyo, Japan: NANO-HITEN - Development of High Strength Hot-rolled Sheet Steel Consisting of Ferrite and Nanometer-sized Carbides (19 Jan 2017)

K. D. Molodov, RWTH Aachen University, Germany: Plasticity in Magnesium: Twinning and Slip Transmission (23 Jan 2017)

M. Hu, RWTH Aachen University, Germany: Phonons beyond Lattice Vibration: From Intrinsic to Atomic Complexity (31 Jan 2017)

A. Stukowski, TU Darmstadt, Germany: From Large-scale Atomistic Simulations to Insights: Powerful Data Analysis and Transformation Tools (06 Feb 2017)

S. Siebentritt, University of Luxembourg, Belvaux, Luxembourg: Solar Cells, Defects and Recombination – News from CIGS (08 Feb 2017)

W. Ludwig, The European Synchrotron ESRF, Grenoble / MATEIS Lab. INSA de Lyon, France: Recent Developments in Synchrotron X-Ray Diffraction Imaging (10 Feb 2017)

D. Dye, Imperial College London, UK: Adventures in Alloys (10 Feb 2017)

R. Woracek, European Spallation Source ESS AB, Lund, Sweden: Probing the Meso- and Macroscale with Advanced Neutron Imaging Techniques (16 Feb 2017)

V. Uhlenwinkel, Institut für Werkstofftechnik, Bremen, Germany: Hot Gas Atomization of Glass Forming Alloys (23 Mar 2017)

D. Trinkle, University of Illinois at Urbana-Champaign, IL, US: Computing Mass Transport in Crystals: Theory, Computation, and Applications (27 Mar 2017, Colloquium)

G. Richter, MPI for Intelligent Systems, Stuttgart, Germany: Filamentary Growth of Magnetic and Alloy Nanowhiskers (28 Mar 2017)

P. Schaaf, TU Ilmenau, Germany: Complex Nanostructures and Nanocomposites for Plasmonic and Photonic Applications (04 Apr 2017, Colloquium)

M. Leitner, Physics Department, TU Munich, Germany: Experimental Determination of Vibrational Dynamics in the Solid State (05 Apr 2017)

B. Cantor, University of Bradford, UK: Multicomponent and High-Entropy Alloys (06 Apr 2017)

B. Berkels, RWTH Aachen University, Germany: Variational Image Processing for Electron Microscopy (12 Apr 2017)

D. Lehmkus, University of Bremen, Germany: Cellular Metals - from Aluminium Foams to Steel Matrix Syntactic Foams (19 Apr 2017)

A. Bergman, Department of Physics and Astronomy, Uppsala University, Sweden and CEA Saclay, France: Atomistic Spin Simulations beyond the Heisenberg Model (26 Apr 2017)

A. Tehranchi, EPFL Lausanne, Switzerland: Atomistic Study of Hydrogen Embrittlement (11 May 2017)

M. G. Willinger, Fritz-Haber-Institut der MPG, Berlin, Germany: The Dynamics of Active Metal Catalysts Revealed by *In Situ* Electron Microscopy (23 May 2017, Colloquium)

J. A. Francis, University of Manchester, UK: Phase Transformation Effects on Residual Stress Development in Welding (13 Jun 2017)

K. Woll, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany: Phase Transformations under Rapid Heating in Metallic Micro- and Nanolaminates (19 Jun 2017)

K. Tschulik, Ruhr-University Bochum, Germany: New Concepts in Electrochemistry – From Magnetic Structuring of Macroscopic Layers to Single Nanoparticle Analysis (28 Jun 2017, Colloquium)

M. J. Demkowicz, Department of Materials Science and Engineering, Texas A&M University, College Station, TX, USA: Some Methods and Applications of Data-driven Inference in Materials Science (29 Jun 2017, Colloquium)

M. G. D. Geers, Technische Universiteit Eindhoven, The Netherlands: Size Effects in Metals: On the Role of Internal Boundaries across the Scales (04 Jul 2017, Colloquium)

S. Ishibashi, AIST, Tsukuba, Japan: Calculation of Positron States and Annihilation Parameters for Vacancy-type Defects (24 Aug 2017)



- M. Militzer*, University of British Columbia, Vancouver, Canada: Next Generation Phase Transformation Models for Advanced Low-carbon Steels (31 Aug 2017)
- K. Chattopadhyay*, Indian Institute of Science, Bangalore, India: Introducing High Temperature Intermetallic Eutectic as Potential Structural Materials (08 Sep 2017)
- A. Bagdasaryan*, Sumy State University, Sumy Oblast, Ukraine: Nitride Coatings based on High-Entropy Alloys (12 Sep 2017)
- N. Sridharan*, Oak Ridge National Labs, USA: Strain Induced Transformations and Additive Manufacturing - A Pathway to Develop Multiphase Materials (14 Sep 2017)
- L. Liliensten*, IRCP Institut de Recherche de Chimie Paris – CNRS-Chimie-Paristech, France: Complex Multicomponent Alloys: Coupled Structural and Mechanical Study of a bcc Model Alloy, and Possible Improvement Path (21 Sep 2017)
- U. Dahmen*, National Center for Electron Microscopy (NCEM), Berkeley, USA: Electron Microscopy of Atomic Structure and Mechanisms in Crystalline Interfaces (05 Oct 2017, 100 years MPIE anniversary colloquium)
- J. Cairney*, University Sydney, Australia: Nanometre-scale Materials Characterisation: New Applications and Techniques (05 Oct 2017, 100 years MPIE anniversary colloquium)
- C. Volkert*, University of Göttingen, Germany: Why So Much Friction? Probing Dissipation at the Nanoscale in Materials with Tailored Electronic and Phononic Degrees of Freedom (05 Oct 2017, 100 years MPIE anniversary colloquium)
- C. Schuh*, Massachusetts Institute of Technology (MIT), Boston, USA: How Grain Boundary Segregation Enables 3D Printing of Bulk Nanostructured Metals (05 Oct 2017, 100 years MPIE anniversary colloquium)
- M. Asta*, University Berkeley, USA: Computational Materials Science: an Enabling Framework for Accelerated Materials Discovery and Design (05 Oct 2017, 100 years MPIE anniversary colloquium)
- P. Gumbsch*, Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany: Triboanalytic and –simulation (05 Oct 2017, 100 years MPIE anniversary colloquium)
- F. Schüth*, Max-Planck-Institut für Kohlenforschung, Mülheim a. d. Ruhr, Germany: Materials Challenges for a Hydrogen Economy (05 Oct 2017, 100 years MPIE anniversary colloquium)
- K. Mayrhofer*, Helmholtz-Institute Erlangen-Nürnberg for Renewable Energy, Erlangen, Germany: Dissolution of Noble Metals and Metal Oxide (05 Oct 2017, 100 years MPIE anniversary colloquium)
- L. Gránásy*, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary: Phase-field Modeling of Polycrystalline Structures: From Needle Crystals to Spherulites (10 Oct 2017, Colloquium)
- P. Junker*, Ruhr-University Bochum, Germany: Variational Methods in Material Modeling: Applications of Hamilton's Principle (10 Oct 2017)
- T. Hyodo*, Innovative Structural Materials Association (ISMA), Tokyo, Japan: Introduction to ISMA (16 Oct 2017)
- T. Murakami*, Kobe Steel LTD., Kobe, Japan: The Influence of Carbon Content Distribution in Retained Austenite on Elongation of TRIP Steel (16 Oct 2017)
- Y. Toji*, JFE Steel Co., Chiba, Japan: High Accuracy Determination of Carbon Content in Steel by FE-EPMA (16 Oct 2017)
- D. Gambino*, Department of Physics, Chemistry, and Biology (IFM), Linköping University, Sweden: Method Development for Defects in Magnetic Materials in the High Temperature Paramagnetic State (17 Oct 2017)
- S. V. Divinski*, Institute of Materials Physics, University of Münster, Germany: Diffusion and Segregation of Solute in Grain Boundaries: From Pure Metals to High-Entropy Alloys (19 Oct 2017)
- P. Denis*, University of Ulm, Germany: Shear Bands in Metallic Glasses: What Are They, How to Find Them? (25 Oct 2017)
- R. E. Sanders, Jr.*, Chongqing University, China, and Novelis Global Research and Technology Center, Kennesaw, GA, USA: Application of Scientific Principles to Aluminium Automotive Sheet (06 Nov 2017)
- B. Appolaire*, Onera, CNRS, Chatillon, France: Insights into the Role of Mechanics on Diffusion-Controlled Phase Transformations using Phase Field Models (07 Nov 2017, Colloquium)
- M. Greiner*, Max-Planck Institute for Chemical Energy Conversion, Mülheim a. d. Ruhr, Germany: Combining Contemporary Methods for a Comprehensive Picture of Functional Materials (13 Nov 2017, Colloquium)
- P. Jenus*, Jožef Stefan Institute, Ljubljana, Slovenia: Synthesis and Characterization of Tungsten-based Composites for High-Temperature Applications (20 Nov 2017)
- S. Betzler*, University of Munich, Germany: Environmental Transmission Electron Microscopy Revealing the Effect of the Atmosphere on the Heat Induced Phase Transformation of Niobium Oxides (24 Nov 2017)
- L. Mädler*, Universität Bremen, Germany: High-Throughput with Particle Technology for Toxicology and Materials Discovery (29 Nov 2017, Reimar Lüst Lecture 2017)



N. Le Biavan, CNRS-CRHEA, Valbonne, France: Zinc Oxide Epitaxial Growth and Optoelectronic Applications (06 Dec 2017)

2018

A. Schneider, CEA Saclay, France: Interplay between magnetic and energetic properties in bcc Fe-Mn alloys from first principles (23 Jan 2018)

C. Stephan-Scherb, Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany: Early Stages of High Temperature Oxidation and Sulphidation Studied by Synchrotron X-Ray Diffraction and Spectroscopy (08 Feb 2018)

B. Curtin, Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, Switzerland: Mechanism of Enhanced Ductility in Mg Alloys (21 Feb 2018, Colloquium)

Y. Champion, Univ. Grenoble Alpes, Grenoble, France: Nanoindentation for Investigating Dynamics of Shear Bands in Metallic Glasses (01 Mar 2018, Colloquium)

B. Klaes, University of Rouen, France: Towards a New 3D Imaging and Analysis Method of Punctual and Clusters Defects in Metals (13 Mar 2018)

P. Chakraborty, S. N. Bose National Centre for Basic Sciences, Kolkata, India: Effect of Hydrogen on Degradation Mechanism of Zirconium: A Molecular Dynamics Study (19 Mar 2018)

M. Krüger, Forschungszentrum Jülich, Institute for Energy and Climate Research, Jülich, Germany: High Temperature Materials - Recent Developments for Future Challenges (17 Apr 2018, Colloquium)

M. T. McDowell, Georgia Institute of Technology/ G. W. Woodruff School of Mechanical Engineering/ School of Materials Science and Engineering - Atlanta, Georgia, USA: *In Situ* Investigation of the Dynamic Evolution of Materials and Interfaces in Energy Storage Systems (19 Apr 2018, Colloquium)

A. Shapeev, Skoltech Innovation Center, Moscow, Russia: Machine-Learning Interatomic Potentials (25 Apr 2018)

K. O'Keeffe, Swansea University, UK: Quantum-Path-Sensitive Extreme Ultraviolet Interferometry (07 May 2018)

J. Grin, MPI for Chemical Physics of Solids, Dresden, Germany: Quantum Chemistry in Position Space and Chemical Bonding in Intermetallic Compounds (08 May 2018, Colloquium)

A. Rollett, Carnegie Mellon Univ., Pittsburgh, PA, USA: Additive Manufacturing, 3D Printing, Porosity and Synchrotron Experiments (14 May 2018)

V. Schnabel, ETH Zürich, Switzerland: Active Materials by Design: Self-healing Metals and Structural Color Sensors with a Thermal Memory (14 May 2018)

R. Kirchheim, Georg-August-Universität Göttingen, Germany: Changing the Interfacial Composition of Carbide and Oxide Precipitates and Its Effect on Hydrogen Trapping (15 May 2018)

R. K. W. Marceau, Deakin University, Geelong, Victoria, Australia: APT Studies of Carbon-related Materials (18 May 2018)

M. Ghidelli, Politecnico di Milano, Milano, Italy: Novel Multifunctional Thin Films with Superior Mechanical and Functional Properties: Advances in Synthesis and Characterization (05 Jun 2018)

L. Stegbauer, Northwestern University, Evanston, IL, USA: Learning from Nature: Investigation of the High-tech Hybrid Nanocomposites of the Chiton Tooth towards 3d-Printable Materials (05 Jun 2018)

A. M. Hodge, University of Southern California, Los Angeles, USA: From Nanometallic Multilayers to Nanostructures: Processes and Mechanisms (06 Jun 2018)

D. Banerjee, Indian Institute of Science, Bangalore, India: Transformations, Recrystallization, Microtexture Texture and Plasticity in Titanium Alloys (08 Jun 2018)

K. Hata, Nippon Steel & Sumitomo Metal Corporation (NSSMC), Japan: Reconstruction of Three-Dimensional Ferrite-Austenite Microstructure and Crystallographic Analysis in an Early Stage of Alpha-Gamma Phase Transformation in Fe-Mn-low C Alloy (15 Jun 2018)

S. Fähler, Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany: Martensitic Microstructure: Modern Art or Science? (19 Jun 2018, Colloquium)

V. Subramanya Sarma, Indian Institute of Technology Madras, Chennai, India: Role of Grain Boundary Character on Hot Corrosion and Liquation Cracking in a Ni Base Superalloy and Austenitic Stainless Steel (22 Jun 2018)

H. Edongue, University of Yaounde I, Cameroon: One-dimensional Simulations of Electrical Properties of $\text{CuIn}_{1-x}\text{Ga}_x\text{Se}_2$ Single Crystal Photo-absorbers (27 Jun 2018)

S. Roy, Indian Institute of Technology, Kharagpur, India: Orientation Dependent Spheroidization Response and α -phase Texture Evolution during Sub β -transus Annealing of Ti-6Al-4V Alloy (04 Jul 2018)



- T. Frolov*, Lawrence Livermore National Laboratory, USA: Predicting Phase Behavior of Grain Boundaries with Evolutionary Algorithms and Machine Learning (09 Jul 2018)
- V. I. Levitas*, Iowa State University, Ames, IA, USA: Phase Field Approach to Phase Transformations, Dislocations, and Their Interaction at Nano- and Microscales (09 Jul 2018)
- U. Hangen*, Bruker Nano GmbH, Aachen, Germany: Streamlined Nanoindentation Workflow for Testing Steels and Alloys: From the Experiment to the Publishable Result (12 Jul 2018)
- T. Sasaki*, National Institute for Materials Science (NIMS), Tsukuba, Japan: Development of Bake-hardenable Wrought Magnesium Alloys for Automotive Body Panel Applications (23 Jul 2018)
- S. Freakley*, Cardiff Catalysis Institute, Cardiff University, Wales, UK: Heterogeneous Catalysis: Not Always Supported Metallic Nanoparticles (25 Jul 2018, Colloquium)
- A. Leineweber*, TU Bergakademie Freiberg, Germany: Iron Nitrides and Carbides: Phase Equilibria, Crystallography, and Phase Transformations (07 Aug 2018, Colloquium)
- T. R. Bieler*, Michigan State University, East Lansing, MI, USA: Quantification and Simulation of Slip Transfer across Grain Boundaries in Near-cube Oriented Aluminum and Mesoscale Elastic Strain Heterogeneity in Titanium (09 Aug 2018)
- T. Berau*, Max Planck Institute for Polymer Research, Mainz, Germany: Multiscale Simulations of Soft Matter Augmented by Data-driven Methods (09 Aug 2018)
- J. Ast*, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland: *In-situ* Deformation and Fracture Experiments at Variable Temperatures in the SEM (23 Aug 2018)
- A. Dollmann*, Karlsruhe Institute of Technology KIT, Germany: High Entropy Alloy CoCrFeMnNi under mild tribological load (30 Aug 2018)
- S. Maier*, RWTH Aachen, Germany: Thermoelectric energy conversion - From waste heat to sustainable energy (11 Sep 2018)
- V. Oliveira*, Federal University of Rio de Janeiro (UFRJ), Brazil: Use of Computational and Physical Simulation on Arc Welding Heat Affected Zone Microstructure Evolution Studies (11 Sep 2018)
- S. Suwas*, Indian Institute of Science, Bangalore, India: Deformation micro-mechanisms and texture evolution in micro-crystalline and nanocrystalline FCC materials: The role of stacking fault energy (19 Sep 2018)
- D. Dini*, Imperial College London, UK: Exploring Surface Interactions at the Molecular Scale in Tribological Applications (25 Sep 2018)
- K. Hemker*, Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD, USA: Topological Optimization and Textile Manufacturing of 3D Lattice Materials (25 Sep 2018)
- S. Barcikowski*, Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany: Metal and Alloy Nanoparticles from Ultrafast, Scalable Laser Synthesis and their Downstream Integration in Catalysis and Additive Manufacturing (02 Oct 2018, Colloquium)
- S. K. Kim*, University of Science and Technology (UST) and Korea Institute of Industrial Technology (KITECH), South Korea: ECO-Almag with no trade-off of strength and ductility: a practical approach to achieve ultra-high strength and ductility (12 Oct 2018)
- C. Ophus*, NCEM, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA: Atomic Electron Tomography Using Coherent and Incoherent Imaging in (Scanning) Transmission Electron Microscopy (18 Oct 2018, Colloquium)
- K. M. Kureh*, Nature Communications, Nature Research, London, UK: How to publish in Nature-branded journals (18 Oct 2018)
- G. Jeffrey Snyder*, Northwestern University, Department of Materials Science and Engineering, Evanston, IL, USA: Complex Thermoelectric Materials (15 Nov 2018)
- A. Baldi*, DIFFER - Dutch Institute for Fundamental Energy Research, Eindhoven, The Netherlands: Hydrogen Storage in Single Metal Nanocrystals (29 Nov 2018, Colloquium)



Lectures and Teaching at Universities

2015 (not included in the Scientific Report 2013 - 2015)

- D. Raabe*, RWTH Aachen: Micromechanics of Materials, WS 2015/2016
M. Rohwerder, Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2015/2016
F. Roters, RWTH Aachen: ICME for Steels, WS 2015/2016
F. Roters, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2015/2016
M. Valtiner, Ruhr-Universität Bochum: Physical Chemistry (joint lecture with C. Morgenstern), WS 2015/2016

2016

- S. Brinckmann*, *R. Janisch*, Ruhr-Universität Bochum: Assessment and Description of Material Properties, WS 2016/17
G. Dehm, Ruhr-Universität Bochum: Mechanische Eigenschaften in kleinen Dimensionen, SS 2016
G. Dehm, *C. Liebscher*, Ruhr-Universität Bochum: Transmissionselektronenmikroskopie für Fortgeschrittene, WS 2016/2017
H.-O. Fabritius, TU München: Bioinspirierte Materialien und Prozesse, WS 2016/2017
B. Grabowski, Universität Paderborn: Computerphysik, WS 2016/2017
T. Hickel, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2016/2017
J. Neugebauer, Ruhr-Universität Bochum: Application and implementation of electronic structure methods, SS 2016
J. Neugebauer, Ruhr-Universität Bochum, IMPRS-SurMat Lecture: Ab Initio Description of Surfaces: Fundamentals and Applications, WS 2016/2017
D. Raabe, RWTH Aachen: Micromechanics of Materials, SS 2016
D. Raabe, RWTH Aachen: Micromechanics of Materials, WS 2016/2017
M. Rohwerder, Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2016/2017
F. Roters, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2016/2017
C. Scheu, RWTH Aachen: Electron Microscopy and Analytical Techniques, WS 2016/2017
H. Springer, RWTH Aachen: Applied micromechanics: multiphase and composite material design, Jun 2016
H. Springer, RWTH Aachen: Micromechanics of Materials Design and micromechanics of metal matrix composites and high-throughput mechanical testing for alloy design, SS 2016
S. Wippermann, Universität Paderborn: Advanced Topics in Quantum Mechanics, WS 2016/2017
S. Zaefferer, Deakin University, Geelong, Australia: Textures, Microstructures and Microscopy, WS 2016/2017
S. Zaefferer, Fachhochschule Münster, Akademie für Elektronenmikroskopie: EBSD – Grundlagen und Anwendungen, Spring Course 2016
S. Zaefferer, *T. Hickel*, *U. Prahl*, RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2016

2017

- S. Brinckmann*, *R. Janisch*, Ruhr-Universität Bochum: Assessment and Description of Material Properties, WS 2017/18
G. Dehm, Ruhr-Universität Bochum: Mechanische Eigenschaften in kleinen Dimensionen, SS 2017
G. Dehm, *C. Liebscher*, Ruhr-Universität Bochum: Transmissionselektronenmikroskopie für Fortgeschrittene, WS 2017/2018
H.-O. Fabritius, TU München: Bioinspirierte Materialien und Prozesse, WS 2017/2018
B. Grabowski, Universität Paderborn: Atomistic Materials Modeling, WS 2017/2018
T. Hickel, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2017/2018



- E. A. Jäggle*, Indian Institute of Technology Roorkee, India: Microstructural Aspects of Additive Manufacturing, Workshop “Microstructural Aspects of Additive Manufacturing”, Dec 2017
- J. Neugebauer*, Ruhr-Universität Bochum, Application and implementation of electronic structure methods, SS 2017
- D. Raabe*, Max-Planck-Institut für Eisenforschung, IMPRS-SurMat Lecture: „Dislocations and crystals, interfaces in materials“ March 2017
- D. Raabe*, RWTH Aachen: Micromechanics of Materials, SS 2017
- D. Raabe*, RWTH Aachen: Micromechanics of Materials, WS 2017/2018
- M. Rohwerder*, Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2017/2018
- M. Rohwerder*, Ruhr-Universität Bochum, IMPRS-SurMat Lecture: „UHV surface analytics“, WS 2017/2018
- M. Rohwerder*, Ruhr-Universität Bochum, IMPRS-SurMat Lecture: “Corrosion”, WS 2017/2018
- F. Roters*, RWTH Aachen, ICME for Steels, SS 2017
- F. Roters*, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2017/2018
- C. Scheu*, RWTH Aachen: Advanced Characterisation, SS 2017
- C. Scheu*, RWTH Aachen: Electron Microscopy and Analytical Techniques, WS 2017/2018
- M. Todorova*, Max-Planck-Institut für Eisenforschung, IMPRS-SurMat Lecture: Phase diagrams and Phase Transformations, SS 2017
- S. Wippermann*, Universität Paderborn: Advanced Topics in Quantum Mechanics, WS 2017/2018
- S. Wippermann*, Max-Planck-Institut für Eisenforschung, IMPRS-SurMat Lecture: “Atomic Structure and Surface Thermodynamics”, Oct 2017
- S. Zaefferer*, Institute of Metals and Technology (IMT), Ljubljana, Slovenia: Textures, Microstructures and Microscopy, Winter Course 2017
- S. Zaefferer*, Fachhochschule Münster, Akademie für Elektronenmikroskopie: EBSD – Grundlagen und Anwendungen, Spring Course, 2017
- S. Zaefferer, T. Hickel, U. Prahl*, RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2017

2018

- S. Brinckmann, R. Spatschek*, RWTH Aachen: Dislocation Dynamics (Software Tools for Integrated Computational Materials Design), SS 2018
- G. Dehm*, Ruhr-Universität Bochum: Mechanische Eigenschaften in kleinen Dimensionen, SS 2018
- G. Dehm, C. Liebscher*, Ruhr-Universität Bochum: Transmissionselektronenmikroskopie für Fortgeschrittene, WS 2018/2019
- T. Hickel*, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2018/2019
- T. Hickel*, Max-Planck-Institut für Eisenforschung, IMPRS-SurMat Lecture: Understanding phase stabilities and microstructure formation with finite temperature ab initio methods, Jun 2018
- J. Neugebauer*, Ruhr-Universität Bochum: Application and implementation of electronic structure methods, SS 2018
- D. Raabe*, RWTH Aachen: Micromechanics of Materials, SS 2018
- C. Scheu*, RWTH Aachen: Advanced Characterisation, SS 2018
- M. Rohwerder*, Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2018/2019
- S. Zaefferer*, Fachhochschule Münster, Akademie für Elektronenmikroskopie: EBSD – Grundlagen und Anwendungen, Spring Course 2018
- S. Zaefferer, T. Hickel, W. Song*, RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2018
- S. Zaefferer*, University of Teheran, Iran: Textures, Microstructures and Microscopy, Autumn Course 2018, Oct 2018



Invited Talks at Conferences and Colloquia

2015 (not included in the Scientific Report 2013 - 2015)

Dehm, G.; Imrich, P. J.; Malyar, N.; Kirchlechner, C.: *Differences in deformation behavior of bicrystalline Cu micropillars containing different grain boundaries*. (Materials Science & Technology (MS&T 2015), symposium entitled "Deformation and Transitions at Grain Boundaries". Columbus, OH, USA. 2015-10-12 to 2015-10-16).

Dehm, G.; Zhang, Z.; Völker, B.: *Structure and strength of metal-ceramic interfaces: New insights by Cs corrected TEM and advances in miniaturized mechanical testing*. (Materials Science & Technology (MS&T 2015), symposium entitled "Structures and Properties of Grain Boundaries: Towards an atomic-scale understanding of ceramics". Columbus, OH, USA. 2015-10-12 to 2015-10-16).

Dehm, G.: *New insights into the mechanical behavior of interface controlled metals*. (Colloquium Materials Modelling, Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF). Universität Stuttgart, Germany. 2015-11-12).

Dehm, G.: *Mikromechanik: lokale Einblicke in die mechanischen Eigenschaften von Materialien*. (Opening of the Christian Doppler Laboratory for Lifetime and Reliability of Interfaces in Complex Multi-Material Electronics „RELAB“. Vienna, Austria. 2015-12-09).

Erbe, A.; Schneider, P.; Sarfraz, A.; Iqbal, D.: *Neue Ergebnisse zur Bildung und Wirkung klassischer und moderner Vorbehandlungen*. (GfKorr Jahrestagung. Frankfurt am Main, Germany. 2015-11-03 to 2015-11-04).

Fabritius, H.-O.: *Photonische Strukturen in der Natur: Wie Lebewesen Licht manipulieren*. (Meilensteintreffen - BMBF Nachwuchsgruppe morPHOX. Universität Paderborn, Germany. 2015-12-16).

Grabowski, B.; Wippermann, S.; Glensk, A.; Hickel, T.; Neugebauer, J.: *Random phase approximation up to the melting point: The impact of anharmonicity and non-local many-body effects on the thermodynamics of Au*. (MISIS Workshop. Moscow, Russia. 2015-10-26 to 2015-10-30).

Grabowski, B.; Ma, D.; Körmann, F.; Neugebauer, J.; Raabe, D.: *Ab initio thermodynamics of the CoCrFeMnNi high entropy alloy: Importance of entropy contributions beyond the configurational one*. (ICAMS Seminar, Ruhr-Universität Bochum, Germany. 2015-11-12).

Grabowski, B.: *Modern materials design from first-principles: Recent progress and future prospects*. (Seminar, Imperial College London, UK. 2015-11-25).

Hickel, T.; Glensk, A.; Zendegani, A.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Ab-initio based assessment of the thermodynamic stability of Al-based intermetallic phases*. (Intermetallics conference. Kloster Banz, Germany. 2015-09-28 to 2015-10-02).

Hickel, T.; Bleskov, I.; Zhang, X.; Körmann, F.; Sandlöbes, S.; Neugebauer, J.: *Ab-initio based understanding of deformation mechanisms in high-Mn steels*. (International Workshop on "Electronic Structure Theory for the Accelerated Design of Structural Materials". Moscow, Russia. 2015-10-26 to 2015-10-30).

Hickel, T.; Glensk, A.; Duff, A.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Ab-initio description of thermodynamic properties of unaries: A progress report*. (Unary SGTE Meeting. Stockholm, Sweden. 2015-11-10).

Hickel, T.; Dutta, B.; Körmann, F.; Neugebauer, J.: *Coupling of magnetic and lattice degrees of freedom in bulk materials*. (P@N seminars, King's College. London, UK. 2015-11-11).

Hickel, T.: *Ab-initio basierte Methoden der mechanismen-orientierten Werkstoffentwicklung*. (8. Nano und Material Symposium Niedersachsen. Salzgitter, Germany. 2015-11-25 to 2015-11-26).

Hickel, T.; Dutta, B.; Glensk, A.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Understanding complex materials at finite temperatures by ab initio methods*. (MRS Fall meeting. Boston, MA, USA. 2015-11-29 to 2015-12-04).

Iqbal, D.; Erbe, A.: *Chemie der kathodischen Delamination – welche Bindung bricht?* (Sitzung des GfKorr Arbeitskreises "Korrosionsschutz durch Beschichtungen". Frankfurt am Main, Germany. 2015-11-03 to 2015-11-04).

Jäggle, E. A.: *Alloys for and by Laser Additive Manufacturing – the basic research perspective*. (2nd European Scientific Steel Panel – Metal Additive Manufacturing, Steel Institute VdEH. Düsseldorf, Germany. 2015-11-23).

Kirchlechner, C.; Imrich, P. J.; Völker, B.; Jaya, B. N.; Raghavan, R.; Harzer, T. P.; Dehm, G.: *Small Scale Mechanical Testing and its Impact on Materials' Applications*. (Keynote Lecture, 14th International Union of Materials Research Societies-International Conference on Advanced Materials. Jeju Island, South Korea. 2015-10-25 to 2015-10-29).

Körmann, F.; Grabowski, B.; Hickel, T.; Neugebauer, J.: *Temperature-dependent coupling of atomic and magnetic degree of freedom from first-principles*. (Electronic Structure Theory for the Accelerated Design of Structural Materials. Moscow, Russia. 2015-10-26 to 2015-10-30).



Kuzmina, M.; Wang, M.; Herbig, M.; Ponge, D.; Tasan, C. C.; Sandlöbes, S.; Raabe, D.: *Segregation engineering enables nanostructured bulk steels by confined martensite-to-austenite reversion*. (Asia Steel International Conference 2015 (Asia Steel 2015). Yokohama, Japan. 2015-10-05 to 2015-10-08).

Kuzmina, M.; Herbig, M.; Ponge, D.; Stoffers, A.; Sandlöbes, S.; Raabe, D.: *Nanostructuring metallic alloys through confined phase transformations*. (Colloquium Lecture - GDCh (Gesellschaft Deutscher Chemiker). Bielefeld, Germany. 2015-10-29).

Kuzmina, M.; Herbig, M.; Ponge, D.; Stoffers, A.; Sandlöbes, S.; Raabe, D.: *Atomic Scale Analysis of Interfaces: Gibbs Adsorption Revisited*. (Colloquium at Physics Department, Friedrich-Alexander-Universität Erlangen-Nürnberg. Erlangen, Germany. 2015-11-02).

Kuzmina, M.; Herbig, M.; Ponge, D.; Choi, P.-P.; Stoffers, A.; Sandlöbes, S.; Raabe, D.: *Segregation engineering enables nanostructured dual-phase laminates via solute decoration and phase transformation at lattice defects*. (Colloquium lecture at Department of Mechanical Engineering, Technische Universiteit Eindhoven, The Netherlands. 2015-11-26).

Liebscher, C.: *High Resolution (Scanning) Transmission Electron Microscopy*. (MPIE-DLR Workshop. German Aerospace Center (DLR) Cologne, Germany, 2015-10-26).

Lymperakis, L.; Neugebauer, J.: *Interplay of kinetics and thermodynamics of epitaxially grown wide bandgap semiconductors*. (10th Asian-European Conference on Plasma Surface Engineering. Jeju Island, Korea. 2015-09-20 to 2015-09-24).

Mayrhofer, K. J. J.: *Novel in situ in operando methods*. (66th Meeting of the International Society of Electrochemistry, Symposium "Novel in situ in operando methods". Taipei, Taiwan. 2015-10-04 to 2015-10-09).

Neugebauer, J.: *Towards automated toolsets for computing high-precision free energies by ab initio approaches*. (Materials Science & Technology (MS&T 2015). Columbus, OH, USA. 2015-10-04 to 2015-10-08).

Neugebauer, J.: *Design of structural materials by ab initio guided multiscale simulations*. (CMRI Symposium. Sendai, Japan. 2015-10-13 to 2015-10-14).

Neugebauer, J.: *Stand ICMPE in Wissenschaft und Industrie*. (VDI-GME Werkstoffdialog. Maria Laach, Germany. 2015-10-16).

Neugebauer, J.: *Mastering the structural and thermodynamic complexity of modern materials*. (ESTADSM Conference. Moskau, Russia. 2015-10-25 to 2015-10-30).

Neugebauer, J.: *Materials design and discovery on the computer: Prospects and challenges*. (Colloquium at Universität Braunschweig, Germany. 2015-12-15).

Scheu, C.: *Dewetting of epitaxial Al thin films on (0001) single crystalline sapphire substrates*. (Materials Science & Technology (MS&T 2015). Columbus, OH, USA. 2015-10-04 to 2015-10-08).

2016

Brinckmann, S.: *Multiscale Simulations of Microstructure Evolution*. (Fracture & Fatigue, Mikromechanische Materialmodellierung. Technischen Universität Bergakademie Freiberg, Germany. 2016-05).

Cerededa, D.; Diehl, M.; Roters, F.; Raabe, D.; Marian, J.: *Unraveling the temperature dependence of the yield strength in BCC metals from atomistically-informed crystal plasticity calculation*. (Dislocations 2016, Purdue University. West Lafayette, IN, USA. 2016-09-19 to 2016-09-23).

Dehm, G.: *Unexpected stress induced martensite formation in ultra-strong pearlitic steel*. (TMS 2016, Symposium: Advanced Characterization Techniques for Quantifying and Modeling Deformation. Nashville, USA, 2016-02-14 to 2016-02-18).

Dehm, G.: *Deformation and Adhesion of Metallic Thin Films*. (International Conference on Metallurgical Coatings and Thin Films, 43rd ICMCTF. San Diego, CA, USA. 2016-04-25 to 2016-04-29).

Dehm, G.: *Mechanically driven martensite formation in ultra-strong pearlitic steel*. (Thermec 2016. Graz, Austria. 2016-05-29 to 2016-06-03).

Dehm, G.: *Stability of nanocrystalline metals: Cu-Cr as a case study*. (PICS meeting. Marseilles, France. 2016-06-14 to 2016-06-17).

Dehm, G.: *Mechanical Testing at Microscopic Length Scale*. (EMMC 15 - 15th European Mechanics of Materials Conference. Brussels, Belgium. 2016-09-07 to 2016-09-09).

Dehm, G.: *Resolving the interplay of nanostructure and mechanical properties by advanced electron microscopy*. (MSE Conference, Materials Science and Engineering. Darmstadt, Germany. 2016-09-27 to 2016-09-29).

Dehm, G.; Harzer, T. P.; Dennenwaldt, T.; Freysoldt, C.; Liebscher, C.: *Chemical demixing and thermal stability of supersaturated nanocrystalline CuCr alloys: Insights from advanced TEM*. (Materials Science & Technology (MS&T 2016). Salt Lake City, UT, USA. 2016-10-23 to 2016-10-27).

Dehm, G.: *Fracture testing of thin films: insights from synchrotron XRD and micro-cantilever experiments*. (2016 MRS Fall Meeting. Boston, MA, USA. 2016-11-27 to 2016-12-02).

- Diehl, M.; Cereceda, D.; Wong, S. L.; Reuber, J. C.; Roters, F.; Raabe, D.: *From Phenomenological Descriptions to Physics-based Constitutive Models EPSRC Workshop on Multiscale Mechanics of Deformation and Failure in Materials*. (EPSRC Workshop on Multiscale Mechanics of Deformation and Failure in Materials. Aberdeen, Scotland. 2016-11-23).
- Diehl, M.; Shanthraj, P.; Reuber, J. C.; Cereceda, D.; Wong, S. L.; Eisenlohr, P.; Roters, F.; Raabe, D.: *DAMASK - the Düsseldorf Advanced Material Simulation Kit Engineering of Advanced Materials*. ("Engineering of Advanced Materials: Numerische Optimierung basierend auf Vorhersagemodellen" Meeting. Erlangen, Germany. 2016-12-20).
- Djaziri, S.; Li, Y.; Goto, S.; Raabe, D.; Dehm, G.: *Unexpected Stress Induced Martensite Formation in Ultra-strong Pearlitic Steel*. (TMS 2016, Symposium: Advanced Characterization Techniques for Quantifying and Modeling Deformation. Nashville, TN, USA. 2016-02-14 to 2016-02-18).
- Duarte, M. J.: *Chemical analysis at the atomic scale: increasing our knowledge of the materials behavior*. (Talk at CINVESTAV-Unidad Queretaro. Queretaro, Mexico. 2016-03-15).
- Duarte, M. J.; Kostka, A.; Crespo, D.; Dehm, G.; Springer, H.; Aparicio-Fernández, R.; Renner, F. U.: *Tailoring microstructures from amorphous precursors: crystallization and corrosion in Fe-based amorphous alloys*. (EMN Meeting on Metallic Glasses 2016. Kuala Lumpur, Malaysia. 2016-09-12 to 2016-09-16).
- Fabritius, H.-O.; Schwind, B.; Wu, X.: *Broadband reflecting fibers with tailored structures inspired by desert ants*. (SPP 1839 Kick-off and Networking Meeting, Wilhelm-Conrad-Roentgen Campus (Bessy II). Berlin, Germany. 2016-02-26).
- Fabritius, H.-O.; Enax, J.; Wu, X.: *Structure-property relations in biological composite materials: An inspiration source for synthetic materials*. (8th Indo-German Frontiers of Engineering Symposium 2016, Alexander von Humboldt Foundation. Potsdam, Germany. 2016-05-19 to 2016-05-22).
- Gault, B.; De Geuser, F.: *A perspective on the ion projection in field ion & atom probe microscopy*. (Atom Probe Tomography & Microscopy 2016. Gyeongju, South Korea. 2016-06-12 to 2016-06-17).
- Gault, B.; Herbig, M.; Liebscher, C.; Kuzmina, M.; Dehm, G.; Mayer, J.; Ponge, D.; Scheu, C.; Stoffers, A.; Sandlöbes, S.; Neugebauer, J.; Raabe, D.: *Defect Segregation studied by Correlative Atom Probe Tomography and Electron Microscopy*. (Japan-Germany Joint Symposium on Advanced Characterization of Nanostructured Materials for Energy and Environment. Düsseldorf, Germany. 2016-06-29).
- Gault, B.: *Full determination of 3D atomic position by combining APT & EM*. (Scientific Directions for Future TEM, Forschungszentrum Jülich, Germany. 2016-07).
- Gault, B.; Herbig, M.; Povstugar, I.; Liebscher, C.; Kuzmina, M.; Cojocaru-Mirédin, O.; Dehm, G.; Nematollahi, G. A.; Ponge, D.; Scheu, C.; Stoffers, A.; Sandlöbes, S.; Neugebauer, J.; Raabe, D.: *Atoms, ions, electrons: simulated, measured and manipulated*. (Workshop on Scientific Directions for Future Transmission Electron Microscopy. Jülich, Germany. 2016-07-13 to 2016-07-15).
- Gault, B.; Katnagallu, S.: *Atom probe microscopy: a new playground for big data analysis?* (Workshop Big-Data-Driven Materials Science. Ringberg Castle, Kreuth, Germany. 2016-07-27 to 2016-07-30).
- Gault, B.; Herbig, M.; Stoffers, A.; Yao, M.; Cojocaru-Mirédin, O.; Liebscher, C.; Raabe, D.: *Correlative Atom Probe Microscopy: Recent Progress and Possibilities*. (European APT Workshop. St Catherine College, Oxford, UK. 2016-09-21 to 2016-09-23).
- Gault, B.; Stoffers, A.; Cojocaru-Mirédin, O.; Liebscher, C.; Li, Y.; Herbig, M.; Raabe, D.: *Materials for energy generation probed at the nanoscale*. (European Energy Research Alliance Conference 2016, EERA. Birmingham, UK. 2016-11-24 to 2016-11-25).
- Grabowski, B.: *Modern materials design from first-principles: Recent progress and future prospects*. (Spring Meeting of the German Physical Society (DPG). Regensburg, Germany. 2016-03-07 to 2016-03-11).
- Grabowski, B.: *Entwicklung von quantenmechanischen Simulationsmethoden für das Design moderner metallischer Werkstoffe*. (Seminar, Universität Paderborn, Germany. 2016-05-09).
- Grabowski, B.; Rogal, L.; Körmann, F.: *Discovery of an ordered hexagonal superstructure in an Al-Hf-Sc-Ti-Zr high entropy alloy*. (Seminar, University of Münster, Germany. 2016-07-12).
- Hadian, R.: *Grain boundary dynamics* (Seminar, Imperial College London, Thomas-Young Center. London, UK. 2016-11-03).
- Herbig, M.; Kuzmina, M.; Haase, C.; Molodov, D. A.; Marceau, R. K. W.; Gutiérrez-Urrutia, I.; Goto, S.; Zaefferer, S.; Choi, P.-P.; Raabe, D.: *Measurement of grain boundary chemistry and crystallography by atom probe tomography and correlated electron microscopy*. (Thermec 2016. Graz, Austria. 2016-05-29 to 2016-06-03).
- Herbig, M.: *Investigation of Segregation Phenomena in Steels by Correlative Transmission Electron Microscopy and Atom Probe Tomography*. (International Conference on Atom Probe Tomography & Microscopy 2016. Gyeongju, South Korea. 2016-06-12 to 2016-06-17).
- Herbig, M.: *How correlative transmission electron microscopy and atom probe tomography could benefit from a 3D nanobeam diffraction orientation mapping technique*. (Workshop on Scientific Directions for Future Transmission Electron Microscopy. Forschungszentrum Jülich, Germany. 2016-07-14 to 2016-07-16).



- Herbig, M.: *Joint Characterization of Crystallography and Chemistry on the Nanometer Scale by Correlative Electron Microscopy and Atom Probe Tomography*. (Interdisciplinary Symposium on 3D Microscopy. Congress Center, Les Diablerets. Switzerland. 2016-10-18 to 2016-10-21).
- Hickel, T.; Dutta, B.; Glensk, A.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Ab initio predicted phase stabilities of complex materials at finite temperatures*. (Materials Chain Conference. Bochum, Germany. 2016-05-30 to 2016-06-01).
- Hickel, T.; Glensk, A.; Nazarov, R.; Dey, P.; Puchakayala, A.; Grabowski, B.; Neugebauer, J.: *Ab initio thermodynamics of point defects in metals: Hydrogen, vacancies and their interaction*. (2nd International Workshop on Models and Data for Plasma-Materials Interaction in Fusion Devices. Loughborough, UK. 2016-06-22 to 2016-06-24).
- Hickel, T.; Mrovec, M.; DiStefano, D.; Elsässer, C.; McEniry, E.; Nazarov, R.; Neugebauer, J.: *New Insights into H trapping and Diffusion in Metallic Microstructures Obtained from Atomistic Simulations*. (2016 International Hydrogen Conference. Jackson Lake Lodge, Moran, USA. 2016-09-11 to 2016-09-14).
- Hickel, T.; Zhang, X.; Rogal, J.; Neugebauer, J.: *The role of interfaces for structural transformations among austenite, ferrite and cementite in steels*. (Seminar on occasion of the 25th anniversary of OCAS research centre Gent, Belgium. 2016-10-27).
- Hickel, T.; Dutta, B.; Körmann, F.; Zhang, X.; Sözen, H.; Neugebauer, J.: *Coupling of magnetic and lattice degrees of freedom in ab initio materials design*. (Physics Seminar, Warwick, UK. 2016-12-01).
- Jäggle, E. A.: *Precipitation Reactions in Age-Hardenable Alloys During Laser Additive Manufacturing*. (Seminar, EMPA (Eidgenössische Materialprüfungs- und Forschungsanstalt). Dübendorf, Switzerland. 2016-02-05).
- Jäggle, E. A.: *Alloys for Laser Additive Manufacturing: general considerations and precipitation reactions*. (Seminar, Institut für Werkstoff-Forschung, DLR Köln 2016. Köln, Germany. 2016-03-21).
- Jäggle, E. A.: *Small variations in powder composition lead to strong differences in part properties*. (Alloys for Additive Manufacturing Workshop 2016. Düsseldorf, Germany. 2016-07-05).
- Jäggle, E. A.: *Alloy design for Additive Manufacturing*. (DARE Annual Workshop 2016. University of Sheffield, UK. 2016-09-02).
- Jäggle, E. A.: *Atomsondentomographie - Chemische Analyse von Grenzflächen mit sub-nm Auflösung*. (19. Arbeitstagung Angewandte Oberflächenanalytik, Fraunhofer-Institut AWZ. Soest, Germany. 2016-09-06).
- Jäggle, E. A.: *Alloys for Additive Manufacturing*. (Research Seminar, Voestalpine Additive Manufacturing Research Center. Düsseldorf, Germany. 2016-09-23).
- Jäggle, E. A.: *Alloys for Additive Manufacturing*. (Verfahrenstechnisches Kolloquium, Universität Bremen, Germany. 2016-10-20).
- Jäggle, E. A.: *Hot cracking in SLM-produced Inconel 738LC: origins and remedy*. (Materials Science and Technology 2016. Salt Lake City, UT, USA. 2016-10-26).
- Jäggle, E. A.: *Phase transformations in alloys produced by Laser Additive Manufacturing*. (Spezialseminar, Fakultät für Werkstoffwissenschaft und Werkstofftechnologie, TU Bergakademie Freiberg, Germany. 2016-11-02).
- Jäggle, E. A.: *Phase transformation phenomena in additively produced alloys*. (Werkstoffkolloquium 2016, Deutsches Zentrum für Luft- und Raumfahrt Köln, Germany. 2016-12-06).
- Kirchlechner, C.; Malyar, N.; Imrich, P. J.; Dehm, G.: *X-ray μ Laue diffraction to understand plasticity at interfaces*. (Spring Meeting of the German Physical Society (DPG), Regensburg, Germany. 2016-03-06 to 2016-03-11).
- Kirchlechner, C.: *Synchrotron based μ Laue diffraction to probe plasticity at interfaces*. (IRSP 2016, 14th International Conference Reliability and Stress-Related Phenomena in Nanoelectronics – Experiment and Simulation. Dresden, Germany. 2016-05-30 to 2016-06-01).
- Kirchlechner, C.; Malyar, N.; Dehm, G.: *Insights into dislocation grain-boundary interaction by X-ray μ Laue diffraction*. (Dislocations 2016. West Lafayette, IN, USA. 2016-09-19 to 2016-09-23).
- Kirchlechner, C.: *What can you learn from a μ Laue experiment?* (8th International Conference on Multiscale Materials Modeling - MMM 2016. Dijon, France. 2016-10-09 to 2016-10-14).
- Kirchlechner, C.: *Brillantes Licht für unser Leben*. (Kopfsalat - zu Gast bei Max Planck, MPI für Eisenforschung. Düsseldorf, Germany. 2016-10-20).
- Körmann, F.; Grabowski, B.; Hickel, T.; Neugebauer, J.: *Lattice excitations in magnetic alloys: Recent advances in ab initio modeling of coupled spin and atomic fluctuations*. (TMS 2016. Nashville, TN, USA. 2016-02-14 to 2016-02-18).
- Körmann, F.; Alling, B.; Grabowski, B.; Dutta, B.; Hickel, T.; Neugebauer, J.: *Parameter-free Computational Design of Magnetic Materials – Recent Advances in Ab Initio Techniques of Coupled Lattice and Spin Fluctuations*. (MRS Fall Meeting 2016. Boston, MA, USA. 2016-11-26 to 2016-12-02).
- Kuzmina, M.; Gault, B.; Herbig, M.; Ponge, D.; Sandlöbes, S.; Raabe, D.: *From grains to atoms: ping-pong between experiment and simulation for understanding microstructure mechanisms*. (Res Metallica Symposium, Department of Materials Engineering, KU Leuven, The Netherlands. 2016-05-11).

Li, Z.; Raabe, D.; Ponge, D.; Springer, H.; Tasan, C. C.; Sandlöbes, S.: *Designing and understanding novel alloys towards superior properties*. (2016 European Workshop on Materials Design. Grenoble, France. 2016).

Liebscher, C.: *Complex Alloys down to atomic resolution*. (Materials Day. Ruhr-Universität Bochum, Germany. 2016-10-25).

Liebscher, C.: *Correlative atomic resolution STEM and atom probe tomography*. (Workshop on Scientific Directions for Future Transmission Electron Microscopy. Jülich, Germany. 2016-10-25).

Liebscher, C.: *Atomic structure of complex engineering materials and interfaces*. (Seminar Engineering Alloys Group, Imperial College, UK. 2016-11-16).

Lymperakis, L.: *Epitaxial Growth of III-Nitrides: Insights from Density Functional Theory Calculations*. (Seminar, Physics Department, University of Crete, Greece. 2016-07-21).

Lymperakis, L.; Freysoldt, C.; Schulz, T.; Maisel, S.; Albrecht, M.; Neugebauer, J.: *Ordering Phenomena in InGaN Alloys – An Ab-Initio Thermodynamics Study*. (International Workshop on Nitride Semiconductors (IWN 2016). Orlando, FL, USA. 2016-10-02 to 2016-10-07).

Marx, V. M.; Palm, M.: *The wet and hot corrosion behavior of iron aluminides*. (THERMEC 2016 – Int. Conf. on Processing & Manufacturing of Advanced Materials. Graz, Austria. 2016-05-29 to 2016-06-03).

Mayrhofer, K. J. J.: *In-situ investigation of catalyst degradation*. (Keynote Lecture, 18th Topical Meeting of the International Society of Electrochemistry. Gwangju, South Korea. 2016-03-08 to 2016-03-11).

Mayrhofer, K. J. J.: *Electrochemical Energy Conversion – the key for sustainable utilization of solar energy*. (Keynote Lecture, Integration of Sustainable Energy Conference (iSEneC). Nürnberg, Germany. 2016-07-11 to 2016-07-12).

Neugebauer, J.: *Mechanical properties and finite temperatures*. (CECAM Conference Lausanne. Switzerland, 2016-01-25 to 2016-01-27).

Neugebauer, J.: *Describing Hydrogen Embrittlement by ab initio guided multiscale modeling – status, perspectives and challenges*. (I²CNER Annual Symposium: Computational Solutions to Fundamental Problems in Carbon-Neutral Energy Research. Fukuoka, Japan. 2016-02-01 to 2016-02-02).

Neugebauer, J.; Glensk, A.; Grabowski, B.; Hickel, T.; Körmann, F.: *Ab Initio thermodynamics: Understanding the fundamental mechanisms behind H embrittlement in metals: An ab initio guided multiscale approach*. (Hydrogenius Workshop. Fukuoka, Japan. 2016-02-03 to 2016-02-04).

Neugebauer, J.: *Understanding the fundamental mechanisms behind H embrittlement in metals: An ab initio guided multiscale approach*. (Joint Hydrogenius and I²CNER International Workshop on Hydrogen-Materials Interactions. Kyushu University, Fukuoka, Japan. 2016-02-04).

Neugebauer, J.; Glensk, A.; Grabowski, B.; Hickel, T.: *Inclusion of Phonon-Phonon and Magnon-Phonon couplings in the thermodynamic description of materials: An ab initio approach*. (Hume-Rothery Award Symposium, TMS 2016. Nashville, TN, USA. 2016-02-14 to 2016-02-19).

Neugebauer, J.: *The digital transformation in Materials Science from a Modellers Perspective*. (VDI Workshop „Digitale Transformation in der Werkstofftechnik“. Düsseldorf, Germany. 2016-02-24).

Neugebauer, J.: *Database concepts and ICME links for atomistic simulations*. (Plenary talk, 2nd International Workshop on Software Solutions for Integrated Computational Materials Engineering ICME 2016. Barcelona, Spain. 2016-04-12 to 2016-04-15).

Neugebauer, J.; Grabowski, B.; Hickel, T.; Ruban, A.V.; Gong, Y.; Reed, R.C.; Koermann, F.: *Ab initio determination of lattice stabilities and comparison to CALPHAD*. (Plenary talk, CALPHAD XLV Conference. Awaji Island, Japan. 2016-05-29 to 2016-06-03).

Neugebauer, J.: *Hydrogen embrittlement research at the MPIE. (Max-Planck-Institut für Eisenforschung)*. (SNEAC Workshop Environmental Assisted Cracking. Trondheim, Norway. 2016-06-08 to 2016-06-10).

Neugebauer, J.: *HPC-Based Quantum Mechanical Design of Engineering Materials*. (Exascale Computing Workshop during ICS 2016. Frankfurt, Germany. 2016-06-19 to 2016-06-23).

Neugebauer, J.: *Ab initio description of defects in materials under extreme conditions*. (2016 Joint ICTP-CAS-IAEA School and Workshop on Plasma-Material Interaction in Fusion Devices. Hefei, China. 2016-07-18 to 2016-07-22).

Neugebauer, J.: *Stahl: Wie ein alter Werkstoff sich immer wieder neu erfindet und damit Wissenschaft und Wirtschaft beflügelt*. (Plenary talk, 129. Versammlung der Gesellschaft der deutschen Naturforscher und Ärzte. Greifswald, Germany. 2016-09-09 to 2016-09-12).

Neugebauer, J.; Glensk, A.; Körmann, F.; Grabowski, B.; Hickel, T.: *Ab initio thermodynamic description of advanced structural materials: Status and challenges*. (Plenary talk, Workshop “Ab-initio Based Modeling of Advanced Materials”. Yekaterinburg, Russia. 2016-09-22 to 2016-09-24).

Neugebauer, J.; Glensk, A.; Grabowski, B.; Hickel, T.: *Modelling structural materials in extreme environments by ab initio guided multiscale simulations*. (International Workshop “Theory and Modelling of Materials in Extreme Environment”. Abingdon, UK. 2016-09-25 to 2016-09-28).



- Neugebauer, J.: *Collective variable description of crystal anharmonicity*. (IPAM Workshop II: Collective Variables in Classical Mechanics. Los Angeles, CA, USA. 2016-10-24 to 2016-10-28).
- Neugebauer, J.; Glensk, A.; Grabowski, B.; Hickel, T.: *Point Defects at Finite Temperatures*. (Bunsen Colloquium - Defects and Diffusion in Solids. RWTH Aachen, Germany. 2016-11-10 to 2016-11-11).
- Neugebauer, J.; Todorova, M.: *Solvent-controlled single atom dissolution, surface alloying and Wulff shapes of nanoclusters; Electrocatalysis at electrocodes in the dry*. (RESOLV Workshop Research Area III, ZEMOS. Bochum, Germany. 2016-11-24).
- Palm, M.: *Development and processing of advanced iron aluminide alloys for application at high temperatures*. (62. Metallkunde Kolloquium. Lech am Arlberg, Austria. 2016-04-11 to 2016-04-13).
- Ponge, D.; Sandlöbes, S.; Millán, S. J.; Choi, P.-P.; Wang, M.; Inden, G.; Dmitrieva, O.; Kuzmina, M.; Herbig, M.; Raabe, D.: *Segregation engineering in medium manganese steels*. (Workshop Integrated Computational Grain Boundary Engineering: The role of segregation. Graz, Austria. 2016-05-29).
- Ponge, D.; Kuzmina, M.; Sandlöbes, S.; Herbig, M.; Raabe, D.: *Austenite formation along dislocations in medium manganese steels*. (Thermec 2016, Intl. Conf. on Processing & Manufacturing of Advanced Materials. Graz, Austria. 2016-05-29 to 2016-06-03).
- Ponge, D.; Roters, F.; Diehl, M.; Shanthyraj, P.; Herbig, M.; Tasan, C. C.; Raabe, D.: *Integrated experimental and simulation analysis of lattice defects and micromechanics in steels*. (Materials Modeling Colloquium, Universität Stuttgart, Germany. 2016-06-23).
- Ponge, D.; Gault, B.; Herbig, M.; Liebscher, C.; Kuzmina, M.; Dehm, G.; Welsch, E. D.; Yao, M.; Hickel, T.; Li, Z.; Tasan, C. C.; Neugebauer, J.; Scheu, C.; Stoffers, A.; Sandlöbes, S.; Raabe, D.: *Chemo-Mechanics at Lattice Defects: from Mechanisms to Bulk Alloys*. (Gordon Research Conference on Thin Film & Small Scale Mechanical Behavior. Lewiston, ME, USA. 2016-07-24 to 2016-07-29).
- Ponge, D.; Wang, M.; Dutta, A.; Kwiatkowski da Silva, A.; Sandlöbes, S.; Millán, S. J.; Choi, P.-P.; Tasan, C. C.; Leyson, G. P. M.; Inden, G.; Dmitrieva, O.; Kuzmina, M.; Herbig, M.; Raabe, D.: *Austenite Reversion in Medium Manganese Steels*. (The 3rd International Conference on High Manganese Steels. Chengdu, China. 2016-11-16 to 2016-11-18).
- Ponge, D.; Kuzmina, M.; Herbig, M.; Sandlöbes, S.; Raabe, D.: *Segregation and Austenite Reversion at Dislocations in a Binary Fe-9%Mn Steel Studied by Correlative TEM-atom Probe Tomography*. (The 3rd International Conference on High Manganese Steels. Chengdu, China. 2016-11-16 to 2016-11-18).
- Raabe, D.: *Materials Engineering through the Ages: from the Battle of Kadesh to Atomic Scale Materials Design*. (Elite Network of Bavaria (ENB) Forum in Erlangen: Focus on Materials Engineering. Erlangen, Germany. 2016-05-30).
- Raabe, D.; Choi, P.-P.; Gault, B.; Ponge, D.; Yao, M.; Herbig, M.: *Segregation engineering for self-organized nanostructuring of materials - from atoms to properties?* (APT&M 2016 - Atom Probe Tomography & Microscopy 2016 (55th IFES). Gyeongju, South Korea. 2016-06-12 to 2016-06-17).
- Raabe, D.; Ponge, D.; Gault, B.; Herbig, M.; Liebscher, C.; Dey, P.; Dehm, G.; Welsch, E. D.; Yao, M.; Wong, S. L.; Hickel, T.; Lipinska-Chwalek, M.; Neugebauer, J.; Prahl, U.; Madivala, M.; Scheu, C.; Bleck, W.: *Ab-Initio Guided Design of Twinning Induced Plasticity and Weight Reduced Austenitic Steels*. (MRS Fall Meeting. Boston, MA, USA. 2016-11-27 to 2016-12-02).
- Raabe, D.; Ponge, D.; Gault, B.; Herbig, M.; Liebscher, C.; Kuzmina, M.; Leyson, G.; Wang, M.; Tasan, C. C.; Nematollahi, G. A.; Springer, H.; Belde, M. M.; Neugebauer, J.; Sandlöbes, S.: *Segregation Engineering - Solute Decoration, Complexions and Transformations for Self-Organized Metallurgical Bulk Nanostructures*. (MRS Fall Meeting. Boston, MA, USA. 2016-11-27 to 2016-12-02).
- Raabe, D.; Li, Z.; Tasan, C. C.; Yao, M.; Ma, D.; Grabowski, B.; Körmann, F.; Neugebauer, J.: *Thermodynamics and Mechanical Properties of Non-Equiatomic CoCrFeMnNi Alloys*. (2016 MRS Fall Meeting. Boston, MA, USA. 2016-11-27 to 2016-12-02).
- Rohwerder, M.: *Conducting Polymers for Intelligent Self-Healing Coatings*. (Energy Materials Nanotechnology (EMN) Meeting on Polymer. Hongkong, Hongkong. 2016-01-12 to 2016-01-15).
- Rohwerder, M.: *Characterization of Oxides in the Heat Affected Zone*. (Welding Workshop "Guidelines for use of welded stainless steel in corrosive environments" at TWI, Granta Park. Cambridge, UK. 2016-01-26).
- Rohwerder, M.: *Nanokapseln für den intelligenten Korrosionsschutz – eine kritische Übersicht*. (GfKORR- Nanoskalige Korrosionsschutzsysteme – Anspruch und Wirklichkeit, Dechema. Frankfurt, Germany. 2016-06-02 to 2016-06-03).
- Rohwerder, M.: *Die Rasterkelvinsonde: neue Entwicklungen für die Charakterisierung von Korrosionsschutzbeschichtungen*. (7. Korrosionsschutz-Symposium. Kloster Irsee, Germany. 2016-06-22 to 2016-06-24).
- Rohwerder, M.: *Metal/Nano-Container Composite Coatings for Long-Term Reliable Self-Healing Capability*. (6th Annual World Congress of Nano Science & Technology – Nano S&T 2016. Singapur, Singapur. 2016-10-26 to 2016-10-28).
- Scheu, C.: *Atomic arrangement and defects in Nb₃O₇(OH) and TiO₂ nanoarrays and their effect on functional properties*. (Talk at Institut für Anorganische und Analytische Chemie, Universität Freiburg, Germany. 2016-01-27).

- Scheu, C.: *The role of defects in Nb₃O₇(OH) and TiO₂ nanoarrays*. (Energy Materials Nanotechnology (EMN). Dubrovnik, Croatia. 2016-05-04 to 2016-05-07).
- Scheu, C.: *New insights into HTPEM fuel cells using electron microscopy techniques*. (THERMEC'2016: 9th International Conference on Processing & Manufacturing of Advanced Materials. Graz, Austria. 2016-05-29 to 2016-06-03).
- Scheu, C.: *Interface structure of Kappa-Carbides in high Mn Steels*. (PICS meeting. Luminy, Marseille, France. 2016-06-14 to 2016-06-17).
- Scheu, C.: *Correlative STEM & Atom Probe Tomography (ATP): Insights in the k-carbide/austenite interface*. (Workshop on "New trends in electron microscopy", Ringberg Castle. Kreuth am Tegernsee, Germany. 2016-06-22 to 2016-06-24).
- Scheu, C.: *Insights into structural and functional properties of nano-structured electrodes for energy and fuel generating devices*. (Talk at Helmholtz-Zentrum Geesthacht, Germany. 2016-06-22 to 2016-06-30).
- Scheu, C.: *Transmission electron microscopy – a versatile tool to study the microstructure of HT-PEMFC*. (Materials Science 2016. Atlanta, GA, USA. 2016-09-12 to 2016-09-14).
- Scheu, C.: *Insights into structural and functional properties of Nb₃O₇(OH) and TiO₂ nanoarrays*. (European Materials Research Society's (EMRS) Fall Meeting. Warsaw, Poland. 2016-09-12 to 2016-09-15).
- Scheu, C.: *Thermal stability and phase transformation of nanostructured Nb₃O₇(OH) photocatalyst*. (Materials Science & Technology (MS&T 2016). Salt Lake City, USA. 2016-10-23 to 2016-10-27).
- Schwarz, T.; Choi, P.-P.; Cojocaru-Mirédin, O.; Mousel, M.; Redinger, A.; Siebentritt, S.; Raabe, D.: *Formation of nano-sized Cu–Sn–Se particles in Cu₂ZnSnSe₄ thin-films and their effect on solar cell efficiency*. (Seminar, Katholieke Universiteit Leuven/IMEC, Belgium. 2016-11-16).
- Šlapáková, M.; Stein, F.; Liebscher, C.; Voß, S.; Kumar, S.: *TEM Analysis of Deformation Structure in Fe₂Nb Laves Phase*. (Seminar on Metal Materials. Prague, Czech Republic. 2016-05-18).
- Springer, H.: *Leichtbau durch Kombinatorische Metallurgie und Prozesstechnik*. (VDI Forum Warmmassivumformung. Düsseldorf, Germany. 2016-02-03).
- Stein, F.; Horiuchi, T.: *Discontinuous Precipitation of the Complex Intermetallic Phase Nb₂Co₇ from Supersaturated Co Solid Solution*. (Thermec 2016. Graz, Austria. 2016-05-29 to 2016-06-03).
- Stein, F.: *Stability Competition between Laves Phase Polytypes*. (Seminar, Escola Politécnica da Universidade de São Paulo, Brazil. 2016-09-12).
- Todorova, M.; Vatti, A.K.; Yoo, S.; Neugebauer, J.: *Oxide stability and defect chemistry in an electrochemical environment: an ab initio perspective*. (Workshop 2016 der DFG-Forschergruppe 1376 "Elementary reaction steps in electrocatalysis: Theory meets experiment". Reisenburg, Günzburg, Germany. 2016-05-01 to 2016-05-04).
- Todorova, M.; Vatti, A.K.; Yoo, S.; Neugebauer, J.: *New Insights into Corrosion Mechanisms from Ab Initio Concepts*. (GRC "Corrosion – Aqueous". New London, NH, USA. 2016-07-10 to 2016-07-15).
- Todorova, M.; Neugebauer, J.: *Formation and dissolution of protective oxide layers in a wet electrochemical environment*. (MMM 2016 Conference. Dijon, France. 2016-10-09 to 2016-10-14).
- Valtiner, M.: *Direct measurement of single molecular interaction free energies at solid/liquid interfaces based on non-equilibrium force spectroscopy*. (Colloquium, TU Berlin, Germany. 2016-01-12)
- Valtiner, M.: *Resolving non-specific and specific adhesive interactions of catechols at solid/liquid interfaces at the single molecular scale*. (Keynote talk, AIChE meeting. San Francisco, CA, USA. 2016-11-17)
- Valtiner, M.: *Measuring single molecule interaction free energies and ion structuring at solid/liquid interfaces*. (INM. Saarbrücken, Germany. 2016-12-02)
- Valtiner, M.: *Quantification of Single Molecular Interactions at Solid/Liquid Interfaces*. (Colloquium, Twente University. Twente, The Netherlands. 2016-12-15)
- Wippermann, S.: *Interface-controlled materials for solar energy conversion: semiconducting nanocrystal solids*. (Colloquium, Tsinghua University. Beijing, China. 2016-07)
- Wippermann, S.: *Entropy stabilizes Peierls condensate: phonon-driven charge density wave formation and adatom-induced early condensation*. (IBS conference on surface atomic wires. Pohang, South Korea. 2016-08-29)
- Zaefferer, S.: *Boundary characterisation using correlative ECCI and EBSD*. (ACMM pre-conference workshop, Geelong, Australia. 2016-01-29).
- Zaefferer, S.: *Correlation of 5-parameter GB character with GB properties*. (ACMM pre-conference workshop, Geelong, Australia. 2016-01-29).
- Zaefferer, S.: *Exploring microstructure-property-relationships of crystalline materials by application of diffraction techniques (electron backscatter diffraction, EBSD, and electron channelling, ECCI) in the SEM*. (Australian conference on microscopy and microanalysis. Melbourne, Australia. 2016-01-31 to 2016-02-04).
- Zaefferer, S.: *Introduction to ECCI*. (EBSD Training Tutorial Workshop. Manchester, UK. 2016-03-22 to 2016-03-23).



Zaefferer, S.: *Electron channelling contrast imaging (ECCI) – Recent advances and new applications*. (RMS-EBSD conference. Manchester, UK. 2016-03-23 to 2016-03-25).

Zaefferer, S.: *Electron channelling contrast imaging (ECCI): an amazing tool for observations of crystal lattice defects in bulk samples*. (SCANDEM. Trondheim, Norway. 2017-06-07 to 2016-06-10).

Zaefferer, S.: *Electron backscatter diffraction (EBSD) –possibilities and limits*. (European Mineralogy Union workshop 2016. Vienna, Austria. 2016-06-19 to 2016-06-20).

Zaefferer, S.: *Investigations on the relationship between crystallographic character of grain boundaries and their functional and mechanical properties in various engineering materials*. (24th International conference on materials and technology. Portorož, Slovenia. 2016-09-27 to 2016-09-29).

Zaefferer, S.: *Direkte Beobachtung von Kristalldefekten in Massivproben mittels Electron-Channelling Contrast Imaging (ECCI) im REM*. (Workshop „Von Nano bis Makro“, der EFDS. Dresden, Germany. 2016-11-07 to 2016-11-09).

Zaefferer, S.: *Electron channelling contrast imaging (ECCI) – an amazing tool for observations of crystal lattice defects in bulk samples*. (Micromat IX. Belo Horizonte, Brazil. 2016-11-22 to 2016-11-25).

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Archie, F. M. F.; Zaefferer, S.: *Investigations on the origin of crack initiation and propagation susceptibility of prior austenite grain boundaries in DP and martensitic steels*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Brinckmann, S.; Fink, C.; Dehm, G.: *Severe Microscale Deformation of Pearlite and Cementite*. (2017 MRS Spring Meeting & Exhibits. Phoenix, AZ, USA. 2017-04-17 to 2017-04-21).

Brinckmann, S.: *Microscale Materials Tribology: Severe Deformation of Pearlite*. (Talk at Institut für Konstruktionswissenschaften und Technische Logistik, Technische Universität Wien, Austria. 2017-11).

Brinckmann, S.: *Severe Deformation of Pearlite during Microscale Tribology*. (Talk at Erich Schmid Institute für Materialwissenschaft. Leoben, Austria. 2017-11).

Cojocaru-Mirédin, O.; Schwarz, T.; Mainz, R.; Abou-Ras, D.: *Understanding the defects in Cu(In,Ga)Se₂ solar cell: a correlative microscopy approach*. (Spring Meeting of the German Physical Society (DPG), Dresden, Germany. 2017-03-19 to 2017-03-24).

Dehm, G.; Malyar, N.; Kirchlechner, C.: *Towards probing the barrier strength of grain boundaries for dislocation transmission*. (Electronic Materials and Applications 2017. Orlando, FL, USA. 2017-01-18 to 2017-01-20).

Dehm, G.: *Resolving the interplay of nanostructure and mechanical properties in advanced materials*. (Karlsruher Werkstoffkolloquium im Wintersemester 2016/2017. Karlsruhe, Germany. 2017-02-07).

Dehm, G.; Harzer, T. P.; Liebscher, C.; Raghavan, R.: *High Temperature Plasticity of Cu–Cr Nanolayered and Chemically Nanostructured Cu–Cr Films*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Dehm, G.; Duarte, M. J.: *Structure and Micro-/Nanomechanics of Materials*. (DLR Cologne. Köln, Germany. 2017-05-23).

Dehm, G.; Malyar, N.; Kirchlechner, C.: *Do we understand dislocation transmission through grain boundaries?* (PICS meeting. Luminy, Marseille, France. 2017-05-30 to 2017-06-02).

Dehm, G.: *Resolving the mechanical performance of materials in microelectronic components with μm spatial resolution*. (FIMPART - Frontiers in Materials Processing Applications, Research and Technology. Bordeaux, France. 2017-07-09 to 2017-07-12).

Dehm, G.: *Towards thermally stable nanocrystalline alloys with exceptional strength: Cu–Cr as a case study*. (16th International Conference on Rapidly Quenched and Metastable Materials (RQ16). Leoben, Austria. 2017-08-27 to 2017-09-01).

Dehm, G.: *Aktuelle Einblicke in den Nanokosmos von Werkstoffen*. (Physikalisches Kolloquium, Bergische Universität Wuppertal, Germany. 2017-11-27).

Dey, P.; Timmerscheidt, T.A.; von Appen, J.; Hickel, T.; Dronskowski, R.; Neugebauer, J.: *Ab initio investigation of the interaction of hydrogen with carbides in advanced high-strength steels*. (Southern University of Science and Technology. Shenzhen, China. 2017-03-20).

Diehl, M.; Naunheim, Y.; Morsdorf, L.; An, D.; Roters, F.; Raabe, D.: *Crystal Plasticity Simulations on Real Data: Towards Highly Resolved 3D Microstructures*. (MRS Spring Meeting 2017. Phoenix, Arizona, USA. 2017-04-17 to 2017-04-21).

Duarte, M. J.; Fang, X.; Brinckmann, S.; Dehm, G.: *In-situ nanoindentation of hydrogen bcc Fe–Cr charged surfaces: Current status and future perspectives*. (Frontiers in Material Science & Engineering workshop: Hydrogen Interaction in Metals, MPIE. Düsseldorf, Germany. 2017-04-11).

Dutta, B.; Hickel, T.; Neugebauer, J.: *Ab initio modelling of phase diagrams in magnetic Heusler alloys: achievements and future challenges*. (SUSTech Global Scientists Forum. Shenzhen, China. 2017-03-18 to 2017-03-20).

Dutta, B.; Hickel, T.; Neugebauer, J.: *Finite temperature excitation mechanisms and their coupling in magnetic shape memory alloys*. (The Materials Research Centre (MRC), Indian Institute of Science (IISc). Bangalore, India. 2017-06-27).

- Dutta, B.; Körmann, F.; Hickel, T.; Neugebauer, J.: *Temperature-driven effects in functional materials: Ab initio insights*. (Talk at University Pierre and Marie CURIE (UPMC). Paris, France. 2017-11-21).
- Fabritius, H.-O.; Wu, X.: *Mechanochromic photonic crystals based on cuticular scales of the weevil *Entimus imperialis**. (IOP Conference "Optical Biomimetics". Imperial College London, UK. 2017-02-22).
- Fabritius, H.-O.: *How living organisms manipulate light: Photonic structures in nature*. (Spring School of the SPP 1839 „Tailored Disorder“. Karlsruhe, Germany. 2017-05-15 to 2017-05-17).
- Fabritius, H.-O.: *In-vitro-Untersuchungen zur Wechselwirkung von synthetischen Hydroxylapatit-Partikeln mit der Zahnschmelzoberfläche*. (Biorepair-Symposium. Bielefeld, Germany. 2017-05-20).
- Fabritius, H.-O.: *Broadband reflecting fibers with tailored structures inspired by desert ants*. (SPP 1839 – Retreat. Koblentz, Germany. 2017-09-18 to 2017-09-20).
- Fabritius, H.-O.; Fabritius-Vilpoux, K.; Enax, J.: *Quantitative Interaktion von HAP-Partikeln mit standardisierten Schmelzoberflächen in vitro und ultrastrukturelle Untersuchungen von Milchzähnen*. (Biorepair-Symposium. Bielefeld, Germany. 2017-12-01 to 2017-12-02).
- Freysoldt, C.; Mishra, A.; Neugebauer, J.: *Ab initio simulations of charged surfaces*. (57th Sanibel Meeting. St. Simons Island, GA, USA. 2017-02-19 to 2017-02-24).
- Freysoldt, C.; Mishra, A.; Neugebauer, J.: *Ab initio simulations of charged surfaces*. (Workshop "High electric fields in electrochemistry and atom probe tomography". Ringberg Castle, Kreuth, Germany. 2017-03-29 to 2017-04-01).
- Gault, B.; Dagan, M.; Katnagallu, S.; De Geuser, F.; Vurpillot, F.; Raabe, D.; Moody, M. P.: *Revisiting Field Ion Microscopy*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).
- Gault, B.; De Geuser, F.; Katnagallu, S.; Nematollahi, G. A.; Dagan, M.; Parviainen, S.; Rusitzka, A. K.; Johnson, E.; Sundell, G.; Andersson, M.; Stephenson, L.; Neugebauer, J.; Moody, M. P.; Vurpillot, F.; Raabe, D.: *Reconstructing field ion microscopy and atom probe data*. (Australian Atom Probe Workshop. Magnetic Island, Australia. 2017-06).
- Gault, B.; Chang, Y.; Kwiatkowski da Silva, A.; Zhao, H.; Kontis, P.; Breen, A. J.; Ponge, D.; Raabe, D.: *Interfaces and defect composition at the near-atomic scale*. (MRS Fall Meeting 2017. Boston, MA, USA. 2017-11-26 to 2017-12-01).
- Glensk, A.; Grabowski, B.; Hickel, T.; Neugebauer, J.; Leitner, M.; Neuhaus, J.; Petry, W.: *Ab initio determination of phonon lifetimes up to the melting point*. (EMRS Spring 2017. Strasbourg, France. 2017-05-22 to 2017-05-24).
- Grabowski, B.: *Development and application of quantum mechanics based simulation tools for the design of modern metallic materials*. (Seminar, RWTH Aachen, Germany. 2017-03-14).
- Grabowski, B.: *Data driven engineering of advanced materials: Combining high precision and scale bridging*. (Colloquium, Forschungszentrum Jülich, Germany. 2017-07-20).
- Grabowski, B.: *Knowledge driven engineering of metals: Development and application of ab initio based scale bridging methods*. (Seminar, TU Delft, Netherlands. 2017-12-04).
- Grabowski, B.: *Knowledge driven engineering of materials: Development and application of ab initio based scale bridging methods*. (Seminar, University Stuttgart, Germany. 2017-12-06).
- Hadian, R.: *Complexions and dewetting*. (Keynote talk, Workshop: Mechanics Meets Energy 2017. Ringberg Castle, Germany. 2017-01-08 to 2017-01-12).
- Hadian, R.; Grabowski, B.; Race, C.; Neugebauer, J.: *Atomistic Simulations on Grain Boundary Migration*. (Keynote talk, Materials Science & Technology (MS&T 2017). Pittsburgh, PA, USA. 2017-10-08 to 2017-10-12).
- Hengge, K.: *TEM Tomography: Insights into the degradation of Pt/Ru fuel cell catalysts*. (3D materials characterization at all length scales and its application to iron and steel, MPIE. Düsseldorf, Germany. 2017-08-29).
- Herbig, M.: *Spatially correlated electron microscopy and atom probe tomography*. (Klausurtagung des Erlanger Lehrstuhls für Werkstoffwissenschaften WW1. Erlangen, Germany. 2017-09-27 to 2017-09-29).
- Herbig, M.: *Materials Science Using Correlative Microscopy*. (National Institute for Materials Science (NIMS). Tsukuba, Japan. 2017-11-08).
- Herbig, M.: *Materials Science Using Correlative Microscopy*. (Nippon Steel & Sumitomo Metals Corporation. Kimitsu, Japan. 2017-11-09).
- Herbig, M.: *Materials Science Using Correlative Microscopy*. (JFE steel corporation. Chiba, Japan. 2017-11-10).
- Herbig, M.; Parra, C. D.; Lu, W.; Toji, Y.; Liebscher, C.; Li, Y.; Goto, S.; Dehm, G.; Raabe, D.: *Where does the carbon atom go in steel? – Insights gained by correlative transmission electron microscopy and atom probe tomography*. (International Symposium on Steel Science 2017. Kyoto, Japan. 2017-11-13 to 2017-11-16).
- Herbig, M.: *Atomare Einsichten in Struktur und Zusammensetzung von Stählen durch korrelative Elektronenmikroskopie/ Atomsondentomographie*. (25. Werkstoffkolloquium des Technischen Beirats. Hannover, Germany. 2017-11-24).
- Hickel, T.; Dey, P.; Mrovec, M.; McEniry, E.; Neugebauer, J.: *Ab initio insights into interface in steels: Fundamentals, recent results & outlook*. (Retreat of the SN department, Tegernsee, Germany, 2017-01-09 to 2017-01-12).



- Hickel, T.; McEniry, E.; Dey, P.; Neugebauer, J.; Mrovec, M.; Di Stefano, D.; Elsässer, C.: *The first principles approach: Insights into hydrogen trapping by microstructures in steels*. (Royal Society Discussion Meeting “The challenges of hydrogen and metals”. London, UK. 2017-01-16 to 2017-01-18).
- Hickel, T.; Bleskov, I.; Aydin, U.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Quantum mechanically guided materials design*. (Summer school “Materials 4.0 - The digitally enabled atom to system revolution”. Dresden, Germany. 2017-09-11 to 2017-09-15).
- Jäggle, E. A.: *Phase transformation phenomena in additively produced alloys*. (Seminar „Materials Science and Technology”. Ruhr-Universität Bochum, Germany. 2017).
- Jäggle, E. A.: *Metallische Werkstoffe in der Additiven Fertigung*. (Workshop “Steels for Additive Manufacturing”. Stahlinstitut VDEh, Düsseldorf, Germany. 2017-02-21).
- Jäggle, E. A.: *Alloys for Additive Manufacturing, Alloys by Additive Manufacturing*. (Seminar, Institut für Umformtechnik und Leichtbau, TU Dortmund, Germany. 2017-06-02).
- Jäggle, E. A.: *Alloys for Additive Manufacturing, Alloys by Additive Manufacturing*. (Laser-Kolloquium, Fraunhofer Institut für Lasertechnik. Aachen, Germany. 2017-07-13).
- Jäggle, E. A.: *Alloys for Additive Manufacturing, Alloys by Additive Manufacturing*. (Seminar, Culham Center for Fusion Energy, Oxford, UK. 2017-08-10).
- Jäggle, E. A.: *Exploiting the Intrinsic Heat Treatment during Laser Additive Manufacturing to trigger Precipitation Reactions*. (International Mechanical Engineering Congress & Exposition (IMECE). Tampa, FL, USA. 2017-11-09).
- Jäggle, E. A.: *Alloys for Additive Manufacturing, Alloys by Additive Manufacturing*. (Plenary talk, Advances in Materials & Processing: Challenges and Opportunities. Indian Institute of Technology Roorkee, India. 2017-11-30).
- Jäggle, E. A.: *Additive Manufacturing and 3D Printing - What's beyond the hype?* (Institute Lecture, Indian Institute of Technology Roorkee, India. 2017-12-03).
- Jäggle, E. A.: *Ex-situ and in-situ heat treatment of alloys during Laser Additive Manufacturing*. (AWT Kolloquium, Institut für Werkstofftechnik. Bremen, Germany. 2017-12-13).
- Jaya, B. N.; Kirchlechner, C.; Dehm, G.: *Fracture Behavior of Nanostructured Heavily Cold Drawn Pearlite: Influence of the Interface*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).
- Kirchlechner, C.; Malyar, N.; Peter, N. J.; Dehm, G.; Micha, J.-S.: *New Insights into Plasticity at Grain Boundaries by Nano- and Micromechanics*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).
- Kirchlechner, C.: *Using nano- and micromechanics to understand interface plasticity*. (Hysitron Nanobrücken 2017. University of Manchester, UK. 2017-04-04 to 2017-04-06).
- Kirchlechner, C.: *Insights into dislocation grainboundary interactions by in situ micromechanics*. (Seminar, FAU Erlangen/Nürnberg. Erlangen, Germany. 2017-06-29).
- Kirchlechner, C.; Kirchlechner, I.; Soler, R.; Du, C.; Schneider, J. M.; Dehm, G.: *In situ small scale fracture experiments*. (RQ16, Microstructural Kinetics Group, Department of Materials Science & Metallurgy. Leoben, Austria. 2017-08-27 to 2017-09-01).
- Körmann, F.; Bleskov, I.; Grabowski, B.; Dutta, B.; Hickel, T.; Neugebauer, J.: *Parameter-free Finite-temperature Computations of Stacking Fault Energies for Magnetic Materials*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).
- Li, Z.: *Designing and understanding novel high-entropy alloys towards superior properties*. (Talk at Universität Kassel, Institut für Werkstofftechnik. Kassel, Germany. 2017-06-06).
- Li, Z.; Raabe, D.: *Designing novel high-entropy alloys towards superior properties*. (Frontiers in Materials Processing Applications, Research and Technology (FiMPART'2017). Bordeaux, France. 2017-07-09 to 2017-07-12).
- Liebscher, C.: *Atomic structure and chemistry of complex energy materials and interfaces*. (Seminar, Lawrence Livermore Laboratory, USA. 2017-03-07).
- Liebscher, C.: *Atomic structure and chemistry of complex energy materials and interfaces*. (63. Metallkunde Kolloquium. Lech am Arlberg, Austria. 2017-04-18 – 2017-04-21).
- Liebscher, C.: *Correlative aberration-corrected STEM and 3D-APT study of coherent interfaces in low density steel*. (Symposium on Advanced Mechanical and Microstructural Characterization Methods for SX Ni- and Co-based alloys. Ruhr-Universität Bochum, Germany. 2017-09-14).
- Lymperakis, L.; Freysoldt, C.; Neugebauer, J.: *Elastically frustrated rehybridization of InGaN surfaces: Implications on growth temperature and alloy ordering*. (Spring school on short period superlattices. Warsaw, Poland. 2017-03-21 to 2-17-03-24).
- Lymperakis, L.: *Physics, growth mechanisms, and peculiarities of III-N surfaces from ab-initio*. (Institute for solid state physics, TU Berlin, Germany. 2017-06-28).
- Malyar, N. V.; Imrich, P. J.; Micha, J.-S.; Dehm, G.; Kirchlechner, C.: *Quantifying dislocation slip transfer by in situ micromechanics*. (MRS Fall Meeting 2017. Boston, MA, USA. 2017-11-26 to 2017-12-01).

Marian, J.; Cereceda, D.; Raabe, D.; Roters, F.; Zhao, Y.; Diehl, M.: *Predicting Materials Strength in BCC Alloys using parameter-less mesoscale approaches*. (MRS Spring Meeting 2017. Phoenix, AZ, USA. 2017-04-17 to 2017-04-21).

Mayrhofer, K. J. J.: *Understanding Electrocatalysis in Fuel Cells and Electrolyzers*. (Keynote Lecture, Recent Advances in Renewable Energy Technology, Education City. Doha, Qatar. 2017-04-02 to 2017-04-03).

Mayrhofer, K. J. J.: *High-throughput methods with online analytics – from fundamental electrocatalysis to real applications*. (Keynote Lecture, 6th Regional Symposium on Electrochemistry for South-East Europe. Balatonkenese, Hungary. 2017-06-11 to 2017-06-15).

Neugebauer, J.; Zhang, X.; Körmann, F.; Grabowski, B.; Hickel, T.; Leyson, G.: *Ab Initio Guided Design of High Strength Steels: Where Do We Stand?* (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Neugebauer, J.: *Ab initio guided design of structural materials with superior mechanical properties*. (APS Meeting 2017. New Orleans, LA, USA. 2017-03-13 to 2017-03-17).

Neugebauer, J.: *How to achieve interoperability - a modeler's perspective*. (1st EMMC International Workshop. Wien, Austria. 2017-04-05 to 2017-04-07).

Neugebauer, J.: *From Semiconductors to High-Strength Steels and Back Again*. (10 years of the Laboratory for Photovoltaics & Semiconductor Physics. Luxembourg, Luxembourg. 2017-05-05).

Neugebauer, J.; Aydin, U.; Grabowski, B.; Hickel, T.: *Machine learning as tool to enhance ab initio based alloy design*. (International workshop on machine learning and data analytics in advanced metals processing. Manchester, UK. 2017-05-23).

Neugebauer, J.; Lymperakis, L.; Freysoldt, C.: *Fundamental compositional limitations in the thin film growth of metastable alloys*. (Keynote Lecture, Rapidly Quenched & Metastable Materials 16. Leoben, Austria. 2017-08-29).

Neugebauer, J.; Hickel, T.; Grabowski, B.; Koermann, F.; Janssen, J.: *Modelling structural materials in realistic environments by ab initio thermodynamics*. (EUROMAT 2017. Thessaloniki, Greece. 2017-09-22).

Neugebauer, J.; Hickel, T.; Grabowski, B.; Pei, Z.; Janssen, J.: *Materials Discovery and Design at Finite Temperatures*. (Materials Science & Technology (MS&T 2017). Pittsburgh, PA, USA. 2017-10-09).

Neugebauer, J.: *Free energy sampling strategies for structurally complex materials*. (IPAM Long Program "Complex High-Dimensional Energy Landscapes" (2017-09-11 to 2017-12-15) Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, UCLA. Los Angeles, CA, USA. 2017-10-16 to 2017-10-20).

Neugebauer, J.; Surendralal, S.; Todorova, M.: *A first principles approach to model electrochemical reactions in an electrolytic cell*. (Workshop: The Electrode Potential in Electrochemistry - A Challenge for Electronic Structure Theory Calculations. Schloß Reisingburg, Günzburg, Germany. 2017-11-26 to 2017-11-29).

Palm, M.: *Iron aluminides: Recent Alloy Developments and Industrial Processing*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Peter, N. J.: *Exploring Grain Boundaries: Structure, Chemistry and Nanomechanics*. (Seminar, National Institute for Electron Microscopy. Berkeley, CA, USA. 2017-09-05).

Ponge, D.; Kuzmina, M.; Sandlöbes, S.; Herbig, M.; Raabe, D.: *Austenite Formation along Dislocations in Medium Manganese Steels*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Ponge, D.; Han, J.; Kwiatkowski da Silva, A.; Raabe, D.; Lee, S.-M.; Lee, Y.-K.; Lee, S.-I.; Hwang, B.: *Relationship between Impact Toughness, Prior Austenite Grain Boundaries and Microstructural Morphology in Medium Mn Steel*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Ponge, D.; Kuzmina, M.; Kwiatkowski da Silva, A.; Wang, M.; Sandlöbes, S.; Herbig, M.; Raabe, D.: *Segregation Engineering in Medium Manganese Steels*. (TMS2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Ponge, D.; Tarzimoghadam, Z.; Klöwer, J.; Raabe, D.: *Hydrogen-assisted Failure in Ni-base Superalloy 718 Studied under In-situ Hydrogen Charging: The Role of Localized Deformation in Crack Propagation*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Ponge, D.; Tasan, C. C.; Springer, H.; Koyama, M.; Kuzmina, M.; Wang, M.; Morsdorf, L.; Gault, B.; Seol, J. B.; Liebscher, C.; Yao, M.; Li, Z.; Gutiérrez-Urrutia, I.; Wang, H.; Neugebauer, J.; Scheu, C.; Raabe, D.: *Metastability Alloy Design*. (16th Intern. Conference on Rapidly Quenched and Metastable Materials (RQ16). Leoben, Austria. 2017-08-31).

Ponge, D.; Tasan, C. C.; Springer, H.; Gutiérrez-Urrutia, I.; Koyama, M.; Kuzmina, M.; Wang, M.; Morsdorf, L.; Gault, B.; Seol, J. B.; Choi, P.-P.; Liebscher, C.; Yao, M.; Li, Z.; Wang, H.; Neugebauer, J.; Scheu, C.; Raabe, D.: *1 Billion Tons of Nanostructure - Metastability Alloy Design and Segregation Engineering*. (38th Risø Intern. Symp. Materials Science Advanced Metallic Materials by Microstructural Design. Roskilde, Denmark. 2017-09-04 to 2017-09-08).

Raabe, D.; Gault, B.; Breen, A. J.; Chang, Y.; Yao, M.; Ponge, D.; Herbig, M.; Liebscher, C.; Dehm, G.; Scheu, C.; Stoffers, A.; Neugebauer, J.: *A Brief History of Metals*. (Public Named Max Planck Lecture, MPIE. Düsseldorf, Germany. 2017).

Raabe, D.; Gault, B.; Breen, A. J.; Chang, Y.; Yao, M.; Ponge, D.; Herbig, M.; Liebscher, C.; Dehm, G.; Scheu, C.; Stoffers, A.; Neugebauer, J.: *Atomic Scale Characterization of Complex Materials*. (Physikalisches Kolloquium, Fakultät für Mathematik und Physik, Universität Freiburg, Germany. 2017-02-06).



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Raabe, D.; Gault, B.; Yao, M.; Scheu, C.; Liebscher, C.; Herbig, M.: *Correlated and simulated electron microscopy and atom probe tomography*. (Workshop on Possibilities and Limitations of Quantitative Materials Modeling and Characterization 2017. Bernkastel, Germany. 2017-05-16).

Raabe, D.; Gault, B.; Breen, A. J.; Chang, Y.; Yao, M.; Ponge, D.; Herbig, M.; Liebscher, C.; Tarzimoghadam, Z.; Dehm, G.; Scheu, C.; Stoffers, A.; Neugebauer, J.: *Multiprobe and Multiscale Characterisation of complex Materials*. (Fraunhofer Conference 'The Future of Materials – Materials Future'. Halle, Germany. 2017-06-19).

Raabe, D.: *Seeing Hydrogen*. (2017 Hydrogen Metal Systems Gordon Research Conference, Stonehill College. Easton, MA, USA. 2017-07-16 to 2017-07-21).

Raabe, D.; Tasan, C. C.; Diehl, M.; Yan, D.; Zambaldi, C.; Zaefferer, S.; Shanthraj, P.; Roters, F.: *Integrated experimental and simulation analysis of stress and strain partitioning in dual phase steel*. (Nanomechanical Testing in Materials Research and Development VI. Dubrovnik, Croatia. 2017-10-01 to 2017-10-06).

Raabe, D.; Gault, B.; Breen, A. J.; Chang, Y.; Yao, M.; Ponge, D.; Herbig, M.; Liebscher, C.; Scheu, C.: *Atomic- and multiscale observation of segregation*. (Eindhoven Multiscale Institute (EMI) Symposium, Eindhoven University. Eindhoven, The Netherlands. 2017-10-30 to 2017-10-31).

Raabe, D.; Gault, B.; Breen, A. J.; Yao, M.; Zhao, H.; Ponge, D.; Stoffers, A.: *Textures Studied at Near Atomic-Scale*. (18th International Conference on Textures of Materials (ICOTOM-18). St. George, UT, USA. 2017-11-06 to 2017-11-10).

Rohwerder, M.: *A Novel Potentiometric Approach to a Quantitative Characterization of Oxygen Reduction Kinetics at Buried Interfaces and under Ultrathin Electrolyte Layers*. (Second International Conference on Electrochemical Science and Technology – ICONEST 2017. Indian Institute of Science, Bangalore, India. 2017-08-10 to 2017-08-12).

Rohwerder, M.: *A Novel Potentiometric Approach to a Quantitative Characterization of Oxygen Reduction Kinetics at Buried Interfaces and under Ultrathin Electrolyte Layers*. (ECASIA 2017. Montpellier, France. 2017-09-24 to 2017-09-29).

Rohwerder, M.; Tran, T. H.: *Novel zinc-nanocontainer composite coatings for intelligent corrosion protection*. (11th International Conference on Zinc And Zinc Alloy Coated Steel Sheet - GALVATECH 2017. Tokyo, Japan. 2017-11-12 to 2017-11-16).

Scheu, C.: *In-situ Transmission Electron Microscopy Observation of Heat-Induced Structural Changes of 3D Nb₃O₇(OH) Networks*. (Electronic Materials and Applications 2017 (EMA). Orlando, FL, USA. 2017-01-18 to 2017-01-20).

Scheu, C.: *Grain growth and dewetting of thin Al films on (0001) Al₂O₃ substrates*. (3 Phase, Interface, Component Systems (PICS), Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), France. 2017-05-30 to 2017-06-02).

Scheu, C.: *Structural and functional properties of Nb₃O₇(OH) nanoarrays and their modification via doping and thermal annealing*. (Talk at Institut für Werkstofftechnik, Technische Universität Ilmenau, Germany. 2017-07-26).

Scheu, C.; Betzler, S. B.: *Nb₃O₇(OH) – a promising candidate for photocatalyst: synthesis, nanostructure and functionality*. (International Conference on Functional Nanomaterials and Nanodevices. Budapest, Hungary. 2017-09-24 to 2017-09-25).

Scheu, C.; Hieke, S. W.; Willinger, M. G.; Wang, Z.-J.; Richter, G.; Dehm, G.: *In-situ electron microscopy: Insights in solid state dewetting of epitaxial Al thin films on sapphire*. (13th Multinational Congress on Microscopy. Rovinj, Croatia. 2017-09-26 to 2017-09-29).

Scheu, C.; Hieke, S. W.; Willinger, M. G.; Wang, Z.-J.; Richter, G.; Dehm, G.: *Evolution of faceted voids and fingering instabilities in a model thin film system - Insights by in-situ environmental scanning electron microscopy*. (Symposium - In situ Microscopy with Electrons, X-rays and Scanning Probes. Universität Erlangen-Nürnberg. Erlangen, Germany. 2017-10-09).

Schwarz, T.: *Untersuchung von Defekten in polykristallinen Dünnschichten mittels Atomsondentomographie*. (gmr2 – Gesellschaft für Materialografie Rhein-Ruhr e.V., MPIE. Düsseldorf, Germany. 2017-11-16).

Soler, R.; Venkatesan, S.; Kirchlechner, C.; Dehm, G.; Rainer, H.; Bartosik, M.; Mayrhofer, P. H.: *Can superlattice structures enhance the fracture toughness of ceramic coating?* (TMS 2017. San Diego, CA, USA. 2017-02-27 to 2017-03-03).

Springer, H.; Raabe, D.: *Rapid Alloy Prototyping – High Throughput Bulk Metallurgy at the MPIE*. (Workshop on machine learning and data analytics in advanced metals processing. RollsRoyce Institute Manchester, UK. 2017).

Springer, H.: *Innovative Stähle*. (Handelsblatt Tagung. Düsseldorf, Germany. 2017-02).

Stockem, I.: *The interaction of spin dynamics and lattice vibrations of CrN in the paramagnetic state*. (BifAM Seminar. Bielefeld, Germany. 2017-11-14).

Taniguchi, S.; Soler, R.; Kirchlechner, C.; Liebscher, C.; Taniyama, A.; Dehm, G.: *In-situ TEM Study of Mechanical Size Effects in TiC Strengthened Steels*. (Microscopy & Microanalysis 2017. St. Louis, MO, USA. 2017-08-06 to 2017-08-10).

Todorova, M.; Neugebauer, J.: *From semiconductor defect chemistry to electrochemistry: Gaining new insights from computational physics tools*. (ICCP10 Conference. Macao, China. 2017-01-16 to 2017-01-20).

- Todorova, M.; Neugebauer, J.: *From semiconductor defect chemistry to electrochemistry: Insight into corrosion mechanisms from ab initio concepts*. (57. Sanibel Symposium. St. Simon Island, GA, USA. 2017-02-21).
- Todorova, M.; Vatti A.K.; Yoo, S.; Neugebauer, J.: *Ab initio description of oxides in an electrochemical environment*. (TMS 2017. San Diego, CA, USA. 2017-02-28).
- Todorova, M.: *From weakened chemical bonds to materials breakdown: An ab initio perspective*. (Spring Meeting of the German Physical Society (DPG), Dresden, Germany. 2017-03-19 to 2017-03-24).
- Todorova, M.; Vatti, A.K.; Yoo, S.; Neugebauer, J.: *Ab-initio modelling of electrochemical processes: Challenges and insights*. (Workshop: Fundamental Electrochemistry: Theory Meets Experiment. Lorentz Center, Leiden, Netherlands. 2017-06-26 to 2016 -06-30).
- Todorova, M.; Vatti, A.K.; Yoo, S.; Neugebauer, J.: *Free energy sampling for electrochemical systems*. (Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, UCLA. Los Angeles, CA, USA. 2017-10-16 to 2017-10-20).
- Todorova, M.; Yoo, S.; Neugebauer, J.: *Selective stabilization of polar oxide surfaces in electrochemical environment*. (Workshop: The Electrode Potential in Electrochemistry - A Challenge for Electronic Structure Theory Calculations. Schloß Reisenburg, Günzburg, Germany. 2017-11-26 to 2017-11-29).
- Valtiner, M.: *Combining X-Ray Reflectivity and white light interferometry in a surface forces apparatus*. (DESY4 workshop. Hamburg, Germany. 2017-03-10 to 2017-03-14)
- Valtiner, M.: *In-situ tracking of the dynamic structure evolution in nanometer confined liquids by combining X-Ray Reflectivity and white light interferometry in a surface forces apparatus*. (Keynote talk, TIN'17. Trieste, Italy. 2017-06-25 to 2017-06-30)
- Valtiner, M.: *Dynamic structure evolution in nanometer confined liquids*. (Keynote talk, World Tribology Conference in Beijing, China. 2017-09-17 to 2017-09-22)
- Valtiner, M.: *Peter Mark Memorial Award Lecture*. (65th AVS conference and symposium. Tampa, FL, USA. 2017-10-29 to 2017-11-03)
- Wippermann, S.: *Exotic forms of silicon for photovoltaic applications*. (E-MRS spring meeting. Strasbourg, France. 2017-02)
- Wippermann, S.: *Optical fingerprints of electrochemical solid/liquid interfaces*. (Resolv Klausurtagung. Velen, Germany. 2017-02)
- Wippermann, S.: *Novel silicon phases and nanostructures for solar energy conversion*. (ICFSI-16. Hannover, Germany. 2017-07)
- Wippermann, S.: *Light-Matter Interactions at Interfaces: From Analysis Techniques to Applications in Solar Energy Conversion*. (Workshop "Internal Interfaces – Perspectives and Challenges for Theory". Marburg, Germany. 2017-11)
- Zaefferer, S., An D., Wang Z.: *Experimental investigations on the relationship between crystallographic character of grain boundaries and their functional and mechanical properties in various engineering materials*. (Spring Meeting of the German Physical Society (DPG). Dresden, Germany. 2017-03-20 to 2017-03-24).
- Zaefferer, S.: *Measurement and observation of elastic stresses and plastic strain phenomena at a local scale using SEM-based diffraction techniques*. (DAAD workshop Recent Trends in Advanced Microstructure Characterization. Universität des Saarlandes, Saarbrücken, Germany. 2017-04-03 to 2017-04-05).
- Zaefferer, S.: *Electron channelling contrast imaging (ECCI) For quantitative analysis of crystal lattice defects in bulk samples*. (Canadian Microscopy and Cytometry Symposium. Montreal, Canada. 2017-05-09 to 2017-05-11).
- Zaefferer, S.: *Electron Channelling Contrast Imaging (ECCI): An Amazing Tool for Observations of Crystal Lattice Defects in Bulk Samples*. (M&M 2017. St. Louis, MO, USA. 2017-08-06 to 2017-08-11).
- Zaefferer, S.: *3D materials investigations – an overview on techniques, applications and limi*. (MPIE-workshop 3D Materials characterization on all length scales and its applications to iron and steel. Düsseldorf, Germany. 2017-08-29).
- Zaefferer, S.: *Observation and quantification of elastic and plastic strain using SEM-based diffraction methods*. (Summerschool Micro- and Nanomechanics. Düsseldorf, Germany. 2017-09-11 to 2017-09-15).
- Zaefferer, S., L. Schemmann, G. Stechmann, F. Ram, F. Archie: *Using orientation microscopy to explore the correlation of materials properties and microstructures*. (25th International conference on materials and technology. Portorož, Slovenia. 2017-10-16 to 2017-10-19).
- Zaefferer, S.: *Observation and quantification of elastic and plastic strain using SEM-based diffraction methods, Part 1*. (7th international conference deformation and fracture of materials and nanomaterials. Moscow, Russia. 2017-11-07 to 2017-11-10).
- Zaefferer, S.: *Observation and quantification of elastic and plastic strain using SEM-based diffraction methods, Part 2*. (7th international conference deformation and fracture of materials and nanomaterials. Moscow, Russia. 2017-11-07 to 2017-11-10).



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- Baron, C.; Springer, H.; Raabe, D.: *Design of cost-efficient high modulus steels as innovative lightweight materials*. (Advanced Composite Materials Congress. Stockholm, Sweden. 2018-06-03 to 2018-06-06).
- Brinckmann, S.: *Using Simulations to Investigate the Apparent Fracture Toughness of Microcantilevers*. (STKS-ICAMS-Seminar. Bochum, Germany. 2018-06).
- Brinckmann, S.: *Understanding the fracture toughness for brittle and ductile materials at the microscale*. (Materials Science and Engineering. Darmstadt, Germany. 2018-09-26 to 2018-09-28).
- Dehm, G.: *“Mechanical microscopy”: Resolving the mechanical behavior and underlying mechanisms of materials with high spatial resolution*. (Keynote Lecture, IMEC18 / The 18th Israel Engineering Conference. Dead Sea, Israel. 2018-02-06 to 2018-02-08).
- Dehm, G.: *Advanced TEM/STEM – a powerful tool to guide materials design*. (Inauguration Symposium, Institut für Metallphysik. Rheinisch-Westfälische Universität Münster, Münster, Germany. 2018-02-15).
- Dehm, G.: *Dislocation – grain boundary interactions: Insights and challenges from micromechanical testing*. (3rd Schöntal Symposium on Dislocation- based Plasticity (DFG Forschergruppe FOR 1650). Schöntal, Germany. 2018-02-25 to 2018-03-02).
- Dehm, G.: *Correlating the state and properties of grain boundaries*. (PICS meeting. Luminy/Marseilles, France. 2018-05-22 to 2018-05-25).
- Dehm, G.; Peter, N.J.; Liebscher, C.H.; Kirchlechner, C.: *Ag-induced phase transformation of a sigma 5 grain boundary in copper*. (THERMEC'2018. Paris, France. 2018-07-18 to 2018-07-13).
- Dehm, G.: *Changing material properties by grain-boundary phase transformation*. (Seminar, University of New South Wales, School of Materials Science and Engineering, Sydney, Australia. 2018-09-17).
- Dehm, G.: *Probing the strength and atomic structure of individual grain boundaries in Cu*. (Seminar, The University of Sydney, Faculty of Engineering & Information Technologies, Sydney, Australia. 2018-09-18).
- Dehm, G.: *Probing dislocation - grain boundary interactions and grain boundary phase transformations: New experiments on Cu bicrystals*. (Seminar, Nanyang Technological University, School of Mechanical & Aerospace Engineering, Singapore. 2018-09-21).
- Dehm, G.: *Structure and Nano-/Micromechanics of Materials*. (Seminar, Beijing Institute of Technology, Beijing, China. 2018-09-24).
- Dehm, G.: *Coexistence of different atomic motifs in a <111> Cu tilt grain boundary resolved by STEM*. (3rd Sino-German Symposium on Advanced Electron Microscopy of Interface Structures and Properties of Materials Tsinghua University. Beijing, China. 2018-09-24 to 2018-09-27).
- Dehm, G.: *Plasticity and Stresses in Thin Films*. (GDRi MECANO General School 2018. Cargèse, Corsica, France. 2018-10-02).
- Dey, P.; Hickel, T.; Neugebauer, J.: *Understanding Hydrogen Embrittlement based on ab initio methods*. (Linköping University, Sweden. 2018-02-15).
- Dey, P.: *Materials design based on ab initio methods: Coherent microstructure & its impact on real application*. (TU Delft, Netherlands. 2018-04-05).
- Diehl, M.; Shanthraj, P.; Eisenlohr, P.; Roters, F.; Raabe, D.: *DAMASK – From Crystal Plasticity to Multi-Physics*. (Seminar of the Centre des Matériaux. Paris, France. 2018-06-08).
- Diehl, M.; Shanthraj, P.; Eisenlohr, P.; Roters, F.; Raabe, D.: *DAMASK - Düsseldorf Advanced Material Simulation Kit*. (Seminar of the Department of Mechanical Engineering, Villanova University, PA, USA. 2018-07-19).
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- Dutta, B.; Körmann, F.; Hickel, T.; Neugebauer, J.: *Role of temperature dependent excitations and the coupling between them in functional materials: Ab-initio insights*. (IFM, Linköping University, Sweden. 2018-02-15).
- Fabritius, H.-O.: *Small-scale structure-property relations in biological hard tissues by nanoindentation*. (Indentation 2018. Liège, Belgium. 2018-09-11 to 2018-09-14).
- Fabritius, H.-O.: *Exploring biomimetic oral care concepts using advanced electron microscopy*. (The Goettingen Spirit Summer School “Symposium on mineralization and biometric concepts in dental research.” Göttingen, Germany. 2018-09-18 to 2018-09-19).
- Freysoldt, C.; Mishra, A. Ashton, M.; Neugebauer, J.: *Density-functional modelling of field evaporation*. (Atom probe tomography and microscopy conference 2018. NIST, Gaithersburg, USA. 2018-06-10 to 2018-06-16).

- Garzón-Manjón, A.; Meyer, H.; Grochla, D.; Ludwig, A.; Scheu, C.: *Insights in the structure and composition of nanoparticles for energy applications*. (Advanced Structural and Functional Materials. Krakow, Poland. 2018-08-20 to 2018-08-24).
- Gault, B.; Kontis, P.; Zhao, H.; Kwiatkowski da Silva, A.; Makineni, S. K.; Chang, Y.; Ponge, D.; Raabe, D.: *Segregations at defects and interfaces and their relations to properties*. (TMS 2018. Phoenix, AZ, USA. 2018-03-11 to 2018-03-15).
- Gault, B.; Kontis, P.; Cormier, J.; Raabe, D.: *From systematic characterisation to the next generation of high performance materials*. (THERMEC 2018. Paris, France. 2018-07-08 to 2018-07-13).
- Glensk, A.: *From Thermodynamics to phonon lifetimes: Anharmonic calculations with ab initio accuracy*. (CECAM workshop: Anharmonicity and thermal properties of solids. Paris, France. 2018-01-10 to 2018-01-12).
- Grabowski, B.; Hadian, S.; Nematollahi, A.; Kirchlechner, C.; Dehm, G.; Neugebauer, J.; Ko, W.S.; Jeon, J.B.: *Dislocation-twin boundary interactions in nanoscale Cu bi-crystals: Simulation versus experiment*. (Schöntal Symposium - Dislocation based Plasticity, Schöntal. Germany. 2018-02-26 to 2018-02-01).
- Grabowski, B.; Zhu, L.; Neugebauer, J.: *Efficient and Accurate Computation of Melting Temperatures and Enthalpies and Entropies of Fusion from Ab Initio*. (TMS 2018. Phoenix, USA. 2018-03-12 to 2018-03-15).
- Grabowski, B.: *Knowledge driven engineering of materials: Development and application of ab initio based scale bridging methods*. (Seminar. HSU Hamburg, Germany. 2018-05-18).
- Hadian, R.: *Grain boundary dynamics*. (Multiscale Materials Modeling (MMM 2018). Osaka, Japan 2018-10-28 to 2018-11-02).
- Hengge, K.: *Insight into the degradation of polymer based fuel cells*. (3rd international conference on Battery and Fuel Cell Technology. London, UK. 2018-09-10 to 2018-09-11).
- Herbig, M.; Li, Y.; Kumar, A.; Morsdorf, L.; Qin, Y.; Mayweg, D.; Goto, S.; Sietsma, J.; Petrov, R.; Raabe, D.: *The role of carbon in the formation of white etching cracks*. (THERMEC 2018 Annual Meeting & Exhibition. Paris, France. 2018-07-08 to 2018-07-13).
- Hickel, T.; Neugebauer, J.; Körmann, F.; Grabowski, B.; Todorova, M.: *Modelling Structural Materials in Realistic Environments by Ab Initio Thermodynamics*. (TMS 2018. Phoenix, Arizona. 2018-03-11 to 2018-03-15).
- Hickel, T.; Bleskov, I.; Dey, P.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Strengthening mechanisms in a precipitation hardened high-Mn lightweight steel*. (6th ESISM Workshop on "Fundamental Issues of Structural Materials". Kyoto, Japan. 2018-02-26 to 2018-02-28).
- Hickel, T.; Lochner, F.; Ahn, F.; Eremin, I.: *Electronic properties, low-energy Hamiltonian and superconducting instabilities in CaKFe₄As₄*. (APS March Meeting 2018. Los Angeles, CA. 2018-03-05 to 2018-03-09).
- Hickel, T.; Glensk, A.; Nazarov, R.; Aydin, U.; Hegde, O.; Grabowski, B.; Neugebauer, J.: *Ab initio thermodynamics of point defects in metals: Hydrogen, vacancies and their interaction*. (2018 Joint ICTP-IAEA School and Workshop on Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments. Miramare, Trieste, Italy. 2018-04-16 to 2018-04-20).
- Hickel, T.: *Characterizing complex materials by ab initio methods*. (Abteilungskolloquium 8. Zerstörungsfreie Prüfung. BAM Berlin, Germany, 2018-06-01).
- Hickel, T.; Grabowski, B.; Körmann, F.; Glensk, A.: *Understanding phase stabilities and microstructure formation with finite temperature ab initio methods*. (MPIE Lecture Series. Düsseldorf, Germany. 2018-06-14).
- Hickel, T.; Dey, P.; Dutta, B.; Friak, M.; Neugebauer, J.: *Phase stability and chemical composition of nano precipitates: A first principles study for the example of kappa carbides*. (Thermec2018. Paris, France. 2018-07-09 to 2018-07-13).
- Huber, L.; Grabowski, B.; Neugebauer, J.; Rottler, J.; Militzer, M.: *High-throughput calculations and modelling of solute-GB segregation* (Thermec 2018 Conference. Paris, France. 2018-07-08 to 2018-07-13).
- Jäggle, E. A.: *New steels for and by Additive Manufacturing*. (JFE Steel Research Seminar. Chiba, Japan. 2018-03-15).
- Jäggle, E. A.: *Alloys and Additive Manufacturing: Conflict or Synergy?* (Seminar, IMDEA Madrid. Spain. 2018-05-18).
- Jäggle, E. A.: *Hot cracking in alloys produced by additive manufacturing*. (THERMEC 2018. Paris, France. 2018-07-08 to 2018-07-13).
- Jäggle, E. A.: *Impact of the process gas atmosphere in Laser Additive Manufacturing – desired and undesired effects*. (Alloys for Additive Manufacturing Symposium 2018. Sheffield, UK. 2018-09-03 to 2018-09-04).
- Kirchlechner, C.: *Beyond Hall-Petch: Mechanism based description of dislocation grain-boundary interactions*. (Spring Meeting of the German Physical Society (DPG), Berlin, Germany. 2018-03-11 to 2018-03-16).
- Kirchlechner, C.; Malyar, N. V.; Dehm, G.: *Dislocation - Grain Boundary Interactions Probed by In-Situ Micromechanical Experiments*. (55th Annual Technical Meeting, SES2018. Madrid, Spain. 2018-10-10 to 2018-10-12).



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- Kontis, P.; Makineni, S. K.; Stephenson, L.; Chang, Y.; Cormier, J.; Ponge, D.; Raabe, D.; Gault, B.: *The Role of Atom Probe Tomography on the Development of the Next Generation of High Performance Materials*. (4th International Congress on 3D Materials Science (3DMS 2018). Helsingør (Elsinore), Denmark. 2018-06-10 to 2018-06-13).
- Kühbach, M.; Roters, F.; Imran, M.; Bambach, M.; Breen, A. J.; Gault, B.; Bajaj, P.; Zhao, H.: *Scalable Quantifying of Evolving Descriptive Spatial Statistics in Full-Field Crystal Plasticity and Atom Probe Tomography*. (Institut für Metallkunde und Metallphysik, RWTH Aachen University, Germany. 2018-06-30).
- Lee, S.; Liebscher, C.; Dehm, G.: *In-situ TEM study on deformation behaviors of CrMnFeCoNi single crystal high entropy alloys*. (European Solid Mechanics Conference (ESMC). Bologna, Italy. 2018-07-02 to 2018-07-06).
- Lee, S.; Duarte, M. J.; Soler, R.; Kirchlechner, C.; Liebscher, C.; Oh, S. H.; Dehm, G.: *In-situ TEM Study of Dislocation Plasticity of a Single Crystal FeCoCrMnNi HEA*. (IAMNano 2018, The International Workshop on Advanced and In-situ Microscopies of Functional Nanomaterials and Devices. Hamburg, Germany. 2018-10-14 to 2018-10-17).
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- Li, Z.; Raabe, D.: *Carbon and Nitrogen Co-doping in an Equiatomic High-entropy Alloy*. (TMS 2018. Phoenix, AZ, USA. 2018-03-11 to 2018-03-15).
- Li, Z.; Raabe, D.: *Interstitially alloyed high-entropy alloys with improved mechanical properties*. (THERMEC 2018. Paris, France. 2018-07-08 to 2018-07-13).
- Liebscher, C.: *Complex interfaces at the atomic scale: insights from aberration-corrected STEM*. (Inauguration colloquium Titan Themis G3 300. Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany. 2018-02-15).
- Liebscher, C.: *Experimental insights into atomic scale phase transitions in metallic grain boundaries*. (International Workshop on Grain Boundaries and Dislocations towards High Performance Metals and Alloys. Beijing University of Technology, China. 2018-06-22).
- Liebscher, C.: *Digitalization in materials characterization*, (9. Brazilian-German Frontiers of Science and Technology Symposium. Florianopolis, Brasil, 2018-10-08 to 2018-10-11).
- Liebscher, C.: *Transmission Electron Microscopy: A tool to decipher the atomic structure of complex materials*. (Inauguration ceremony Talos F200X G2, Chair of Nonferrous Metallurgy, Montanuniversität Leoben, Leoben, Austria, 2018-10-31).
- Lymperakis, L.; Freysoldt C.; Neugebauer J.: *Elastically Frustrated Rehybridization: Implications in Alloy Ordering and Strong Compositional Limitations in Epitaxial InGaN Films*. (1st German Austrian Conference of Crystal Growth. Vienna, Austria. 2018-02-14 to 2018-02-16).
- Malyar, N.V.; Micha, J.-S.; Dehm, G.; Kirchlechner C.: *Quantifying dislocation slip transmission by in situ micromechanics* (18th International Conference on the Strength of Materials (ICSMA18). Ohio State University. Columbus, OH, USA. 2018-07-15 to 2018-07-19).
- Malyar, N. V.; Kirchlechner, C.; Dehm, G.: *Dislocation Transmission Through Grain Boundaries: Insights from In-Situ Micromechanical Experiments*. (Materials Science & Technology (MS&T 2018). Columbus, OH, USA. 2018-10-14 to 2018-10-18).
- Molin, J.-B.; Renversade, L.; Malyar, N. V.; Ulrich, O.; Micha, J.-S.; Kirchlechner, C.: *Nondestructive 3D information on dislocation density and elastic strain in deforming micro-fatigue specimen*. (ESMC 2018. Bologna, Italy. 2018-07-02 to 2018-07-06).
- Mouton, I.; Katnagallu, S.; Schwarz, T.; Makineni, S. K.; Printemps, T.; Grenier, A.; Barnes, J. P.; Cojocaru-Mirédin, O.; Raabe, D.; Gault, B.: *Calibration of Atom Probe Tomography Reconstructions from Correlation with Electron Tomograms or Micrographs*. (APT&M 2018, NIST. Gaithersburg, MD, USA. 2018-06-10 to 2018-06-15).
- Neugebauer, J.; Todorova, M.; Grabowski, B.; Hickel, T.; Leyson, G.: *Understanding the fundamental mechanisms behind H embrittlement: An ab initio guided multiscale approach*. (Seminar, E2M (“Wall Forum”). Max-Planck-Institut für Plasmaphysik, Garching, Germany. 2018-02-26).
- Neugebauer, J.; Janssen, J.; Körmann, F.; Grabowski, B.; Hickel, T.: *Exploration of large ab initio data spaces to design structural materials with superior mechanical properties*. (Hume-Rothery Award Symposium, TMS 2018. Phoenix, AZ, USA. 2018-03-11 to 2018-03-15).
- Neugebauer, J.; Zhu, L.-F.; Koermann, F.; Grabowski, B.; Hickel, T.: *From electrons to the design of structurally complex materials*. (SFB ViCoM conference EPT 2018: From electrons to phase transitions. Vienna, Austria. 2018-04-03 to 2018-03-06).
- Neugebauer, J.; Freysoldt, C.; Lymperakis, L.: *Understanding fundamental doping and stoichiometry limits in semiconductors by ab initio modelling*. (Plenary talk, EDS 2018 Conference. Thessaloniki, Greece. 2018-06-24 to 2018-06-29).

Neugebauer, J.; Hadian, S.; Huber, L.; Race, C.; Grabowski, B.: *Modelling thermodynamics and kinetics of general grain boundaries: Challenges and successes* (Thermec 2018 Conference. Paris, France. 2018-07-08 to 2018-07-13).

Neugebauer, J.; Freysoldt, C.: *First-principles approaches for charged defects in low dimensional systems*. (Conference on Physics of Defects in Solids: Quantum Mechanics meets Topology. Trieste, Italy. 2018-07-09 to 2018-07-13).

Neugebauer, J.; Lymperakis, L.; Freysoldt, C.: *Fundamental compositional limitations in the thin film growth of metastable alloys*. (Keynote lecture, 3rd Conference on Advanced Functional Materials. Vildmarkshotellet Kolmården, Norrköping, Sweden. 2018-08-21 to 2018-08-23).

Neugebauer, J.; Zhu, L.; Körmann, F.; Grabowski, B.; Hickel, T.: *Data driven approaches in materials design: theory meets experiment*. (RCTP-2018 Conference. Moscow, Russia. 2018-10-15 to 2018-10-19).

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Neugebauer, J.: *Electronic structure and computational metallurgy*. (Workshop Coupling and linking simulations - EMMC expert meeting and roadmap, CECAM-HQ-EPFL, Lausanne, Switzerland. 2018-11-08 to 2018-11-09).

Neugebauer, J.; Ikeda, Y.; Körmann, F.; Grabowski, B.; Hickel, T.: *High entropy alloys beyond configurational entropy*. (MRS 2018 Conference. Boston, USA. 2018-11-25 to 2018-12-01).

Ponge, D.; Tarzimoghadam, Z.; Klöwer, J.; Raabe, D.: *Hydrogen-assisted Failure in Ni-base Superalloy 718 Studied under In-situ Hydrogen Charging: The Role of Localized Deformation in Crack Propagation*. (Spring Meeting of the German Physical Society (DPG), Berlin, Germany. 2018-03-11 to 2018-03-16).

Ponge, D.; Dutta, A.; Sandlöbes, S.; Raabe, D.: *Strain partitioning in medium manganese steels*. (THERMEC 2018, Intl. Conf. on Processing & Manufacturing of Advanced Materials. Paris, France. 2018-07-09 to 2018-07-13).

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Herbig, M.; Makineni, S. K.; Liebscher, C.; Yao, M.; Scheu, C.; Gault, B.: *Chemo-Mechanics in Metallic Alloys*. (16th Edition of the European Mechanics of Material Conference. Nantes, France. 2018-03-25 to 2018-03-28).

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Rohwerder, M.: *Delamination of organic coatings: unraveling the underlying mechanisms*. (69th Annual Meeting of the International Society of Electrochemistry. Bologna, Italy. 2018-09-02 to 2018-09-07).

Rohwerder, M.: *High-throughput approaches in Corrosion Research by Scanning Flow Cell and Scanning Kelvin Probe*. (2nd Forum of Materials Genome Engineering in Beijing, China. 2018-10-14 to 2018-10-16).

Roters, F.; Sharma, L.; Diehl, M.; Shanthraj, P.: *Including Damage Modelling into Crystal Plasticity Simulations using the Düsseldorf Advanced Material Simulation Kit DAMASK*. (Symposium Nano and Micro Scale Damage in Metals. Utrecht, The Netherlands. 2018-02-08).

Roters, F.; Wong, S. L.; Shanthraj, P.; Diehl, M.; Raabe, D.: *Multi-physics simulation of advanced high strength steels*. (THERMEC 2018. Paris, France. 2018-07-11).

Scheu, C.: *3D Nb₃O₇(OH) Nanoarrays – Structure, Stability and Functional Properties*. (Talk at Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Germany. 2018-01-10).

Scheu, C.: *Defects in AgSbTe₂ thermoelectrics*. (3 Phase, Interface, Component Systems (PICS), Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), France. 2018-05-23 to 2018-05-25).

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- Scheu, C.: *Unraveling the secrets of interfaces and grain boundaries*. (Seminar, University of New South Wales, School of Materials Science and Engineering, Sydney, Australia. 2018-09-17).
- Scheu, C.: *Insights in interfaces by combining Cs corrected STEM and APT experiments with atomistic simulations*. (Seminar, The University of Sydney, Faculty of Engineering & Information Technologies, Sydney, Australia. 2018-09-18).
- Scheu, C.: *Nanostructured photocatalyst based on transition metal oxides*. (Seminar, National University of Singapore, Dept. of Materials Science and Engineering, Singapore. 2018-09-21).
- Scheu, C.: *Insights in the structure and functionality of doped and undoped Nb₃O₇(OH) nanoarrays*. (nanoGe Fall Meeting 2018, Torremolinos, Spain. 2018-10-22 to 2018-10-26).
- Scheu, C.: *Interface characterization of applied materials at ultimate resolution*. (Seminar, Beijing Institute of Technology, Beijing, China. 2018-09-24).
- Scheu, C.: *Degradation analysis of electrocatalyst using identical location STEM measurements*. (3rd Sino-German Symposium on Advanced Electron Microscopy of Interface Structures and Properties of Materials, Tsinghua University, Beijing, China. 2018-09-24 to 2018-09-27).
- Sohn, S. S.; Jo, Y. H.; Choi, W.-M.; Kim, D. G.; Kim, H. S.; Lee B. J.; Lee S.: *Transformation-induced plasticity in HEA: FCC to BCC transformation*. (Thermec 2018, Paris, France. 2018-07-08 to 2018-07-13).
- Todorova, M.; Surendralal, S.; Yoo, S.; Neugebauer, J.: *Atomistic insights into surface stability and reactivity at solid/liquid interfaces from first principles calculations*. (Technical University Vienna, Austria. 2018-04-10).
- Todorova, M.; Surendralal, S.; Yoo, S.; Neugebauer, J.: *Insights into corrosion mechanisms from ab initio calculations*. (BASF "Corrosion Forum", Ludwigshafen, Germany. 2018-04-24).
- Todorova, M.; Neugebauer, J.: *Insights into electrochemical problems from the perspective of semiconductor defect chemistry*. (Tutorial Lecture, International Workshop on Computational Electrochemistry (IWCE), Aalto University, Helsinki, Finland, 2018-07-09).
- Todorova, M.; Yoo, S.; Surendralal, S.; Neugebauer, J.: *Stability and reactivity of solid/liquid interfaces from ab initio calculations*. (International Workshop on Computational Electrochemistry (IWCE), Aalto University, Helsinki, Finland. 2018-07-10 to 2018-07-12).
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- Todorova, M.; Vatti, A.K.; Yoo, S.; Surendralal, S.; Neugebauer, J.: *From semiconductor defect chemistry to electrochemistry: Challenges and insights*. (Keynote talk, AMaSiS 2018 Workshop, Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany. 2018-10-08 to 2018-10-10).
- Soler, R.; Gleich, S.; Fager, H.; Achenbach, J.O.; Kirchlechner, C.; Schneider, J.M.; Scheu, C.; Dehm, G.: *Mo₂BC thin films - a material system combining hardness and ductility?* (Keynote Lecture, 5th European Conference in Nanofilms ECNF2018, Cranfield University, Cranfield, UK. 2018-03-20 to 2018-03-22).
- Stein, F.: *Microstructure Design from Liquidus Surfaces - The Value of Phase Diagrams for Materials Development*. (64th Metal Research Colloquium, Department for Metal Research and Materials Testing of the Montanuniversität Leoben, Lech am Arlberg, Austria. 2018-04-09 to 2018-04-11).
- Stein, F.; Takaja, S.; Vogel, S. C.: *On the Structure and Stability of the γ Brass-type High-temperature Phase in Al-rich Fe-Al(-Mo) Alloys*. (TOFA 2018, Discussion Meeting on Thermodynamics of Alloys, Seoul, South Korea. 2018-10-01 to 2018-10-05).
- Uebel, M.: *Redox-responsive coatings for smart corrosion protection: how to design highly responsive coatings?* (AMI's Self-Healing Polymers 2018, London, UK. 2018-10-08 to 2018-10-09).
- Valtiner, M.: *Interfacial Structuring of Ionic Liquids in the Presence of Water: From Neat Liquids to Aqueous Solutions*. (Gordon Conference Aqueous Solutions and Electrolytes, Holderness, NH, USA. 2018-07-23 to 2018-07-28).
- Waseda, O.: *Machine-Learning assisted Heisenberg model for systems with ill-defined magnetic interactions*. (Thermec 2018 Conference, Paris, France. 2018-07-08 to 2018-07-13).
- Wippermann, S.: *Modeling electrochemical solid/liquid interfaces from first principles*. (Materialforschungstag Mittelhessen, Marburg, Germany. 2018-05).
- Wippermann, S.: *Modeling electrochemical solid/liquid interfaces from first principles*. (IEEE Nano, Cork, Ireland. 2018-07).
- Wippermann, S.: *Ab initio molecular dynamics simulations at constant electrode potential*. (Colloquium KIT, Karlsruhe, Germany. 2018-11).
- Zavašnik, J.: *Beyond beautiful pictures: nanowires, nanotubes and nanoparticles in Transmission Electron Microscope*. (Talk at Zentrum für molekulare Spektroskopie und Simulation solvensgesteuerter Prozesse (ZEMOS), Fakultät für Chemie und Biochemie, Ruhr-Universität Bochum, Germany. 2018-08-02).



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Zaefferer, S.: *Understanding the correlation of crystallographic character and corrosion behaviour of grain boundaries in a stainless steel using large-area 3D EBSD.* (RMS-EBSD conference. Plymouth, UK. 2018-04-10 to 2018-04-11).

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Habilitation, Doctoral, Diploma, Master and Bachelor Theses

Habilitation Theses

2016

PD Dr. rer. nat. M. Rohwerder: Wasserstoff in Metallen: neue Messverfahren zum Nachweis mit hoher räumlicher Auflösung (Ruhr-Universität Bochum)

2018

Dr. rer. mont. C. Kirchlechner: Dislocation Slip Transfer Mechanisms: Quantitative Insights from *in situ* Micromechanical Testing (Montanuniversität Leoben)

PD Dr.-Ing. H. Springer: Integrated Alloy and Processing Design of High Modulus Steels (RWTH Aachen)

Doctoral Theses

2015 (not included in the Scientific Report 2013 - 2015)

Dr.-Ing. C. Begau: Characterization of crystal defects during molecular dynamics simulations of mechanical deformation (Ruhr-University Bochum)

Dr. rer. nat. S. Betzler: 3D Hierarchical Nb₃O₇(OH) Superstructures: Synthesis, Structural Characterization and Photophysical Properties (LMU München), **with distinction “summa cum laude”**

Dr. rer. nat. A. Müller: Transmission Electron Microscopic Investigation of Several Nanostructured Photoelectrodes for Photoelectrochemical Water Splitting (LMU München)

Dr.-Ing. J. Nellessen: Effects of strain amplitude, cycle number and orientation on low cycle fatigue microstructures in austenitic stainless steel and aluminum (RWTH Aachen)

Dr.-Ing. V. Schnabel: Stiff and damage-tolerant metallic glasses (RWTH Aachen), **with distinction “summa cum laude”**

Dr.-Ing. M. Wang: Nanolaminate TRIP-TWIP martensite matrix steels: Design and Characterization (RWTH Aachen)

Dr.-Ing. D. Yan: Micromechanically guided design of graded ultrafine-grained dual-phase steel (Ruhr-Universität Bochum)

2016

Dr. rer. nat. M. von Avenarius: Mechanical properties in metallic glasses and their deformation mechanisms (RWTH Aachen)

Dr. rer. nat. U. Aydin: Interstitial solution enthalpies derived from first-principles: Knowledge Discovery using High-Throughput Databases (Universität Paderborn)

Dr.-Ing. V. S. P. K. Bhogireddy: Liquid metal induced grain boundary embrittlement: A multi-scale study (Ruhr-Universität Bochum)

Dr. rer. nat. C. D. Fernández Solís: Application of biopolymer-organosiloxane hybrid films as protective barrier on metallic surfaces (Ruhr-Universität Bochum)

Dr. rer. nat. J.-P. Grote: Design of a Novel Electrochemical Activity and Selectivity Analysis Instrument (Ruhr-Universität Bochum)

Dr.-Ing. T. P. Harzer: Nanostructure, thermal stability and mechanical properties of vapor phase deposited supersaturated Cu–Cr thin film alloys (Ruhr-Universität Bochum)



- Dr.-Ing. M. Lai:* Experimental-theoretical study of the interplay between deformation mechanisms and secondary phases in metastable β titanium alloys (RWTH Aachen)
- Dr. rer. nat. M. M. Lange:* The microstructural impact on high temperature corrosion in DMV 617 mod under coal-fired conditions (RWTH Aachen)
- Dr.-Ing. X. Li:* Al-rich Fe–Al based alloys: Phase equilibria, microstructures, coarsening kinetics and mechanical behavior (Ruhr-Universität Bochum)
- Dr.-Ing. V. M. Marx:* The mechanical behavior of thin metallic films on flexible polymer substrate (Ruhr-Universität Bochum)
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- Dr.-Ing. B. Philippi:* Micromechanical characterization of lead-free solder and its individual microstructure elements (Ruhr-Universität Bochum)
- Dr.-Ing. F. Ram:* The Kikuchi bandlet method for the intensity analysis of the Electron Backscatter Kikuchi Diffraction Patterns (RWTH Aachen), **with distinction „summa cum laude“**
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- Dr.-Ing. X. Wu:* Elementary deformation processes during low temperature and high stress creep of Ni-base single crystal superalloys (Ruhr-Universität Bochum)
- Dr.-Ing. J. Zhang:* Microstructure design via site-specific control of recrystallization and nano-precipitation (RWTH Aachen)

2017

- Dr. rer. nat. A. Altin:* Cyclodextrin for Zinc Corrosion Protection (Ruhr-Universität Bochum)
- Dr.-Ing. C. Baron:* On the design of alloys and synthesis for composite steels (RWTH Aachen)
- Dr. Eng. D. J. Bowden:* Assessment of Co-free hardfacing stainless steel alloys for nuclear applications (Manchester University, UK)
- Dr. rer. nat. H.-W. Cheng:* Probing the Solid/Liquid Interfacial Structure of Ionic Liquids and Battery Fluids by Surface Force Measurements: Influence of water, ions and surface chemistry in interfacial structuring (Ruhr-Universität Bochum), **with distinction "summa cum laude"**
- Dr.-Ing. V. Dandapani:* Hydrogen Permeation based Potentiometry as a New Quantification Tool for Electrochemical Reactivity at Buried Interfaces and under Nanoscopic Electrolyte Layers (Ruhr-Universität Bochum)
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- Dr. rer. nat. S. Gleich:* Investigation of Sputtered Mo₂BC Hard Coatings: Correlation of Nanostructure and Mechanical Properties (RWTH Aachen)



Dr. rer. nat. K. A. Hengge: Investigation of alternative catalyst and support materials and their effect on degradation in high-temperature polymer-electrolyte-membrane fuel cells (RWTH Aachen), **with distinction "summa cum laude"**

Dr. rer. nat. S. W. Hieke: Solid state dewetting phenomena of aluminum thin films on single crystalline sapphire (RWTH Aachen)

Dr. rer. nat. A. Koprek: Element redistribution and defect formation at the CdS/CIGS interface (RWTH Aachen)

Dr.-Ing. N. V. Malyar: Dislocation transmission through copper grain boundaries at the micron scale (Ruhr-Universität Bochum)

Dr.-Ing. K. D. Molodov: Investigation of deformation mechanisms in magnesium crystals (RWTH Aachen)

Dr.-Ing. L. Morsdorf: Fundamentals of ferrous low-carbon lath martensite: from the as-quenched, to tempered and deformed states (RWTH Aachen)

Dr.-Ing. E. Pizzutilo: Towards On-Site Production of Hydrogen Peroxide with Gold-Palladium catalysts in Electrocatalysis and Heterogeneous Catalysis (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

Dr.-Ing. G. Polymeros: Performance of catalysts in electrode structure – bridging the gap between fundamental catalyst properties and behavior in real applications (Ruhr-Universität Bochum)

Dr.-Ing. G. Stechmann: A Study on the Microstructure Formation Mechanisms and Functional Properties of CdTe Thin Film Solar Cells Using Correlative Electron Microscopy and Atomistic Simulations (RWTH Aachen)

Dr. rer. nat. A. Stoffers: Grain boundary segregation in multicrystalline Silicon studied by correlative microscopy (RWTH Aachen)

Dr.-Ing. M. Stricker: Die Übertragung von mikrostrukturellen Eigenschaften aus der diskreten Versetzungsdynamik in Kontinuumsbeschreibungen (KIT, Karlsruhe)

Dr.-Ing. Z. Tarzimoghadam: An investigation of hydrogen/microstructure interaction in complex nickel-based alloys: Multi-scale detection and embrittlement mechanisms (RWTH Aachen)

Dr.-Ing. C. Toparli: Passivity and passivity breakdown on copper: In situ and operando observation of surface oxides (Ruhr-Universität Bochum)

Dr.-Ing. T. H. Tran: Regenerative Nanocomposite-Coatings tailored for Smart Corrosion Protection (Ruhr-Universität Bochum)

Dr.-Ing. Z. Wang: Investigation of crystallographic character and molten-salt-corrosion properties of grain boundaries in a stainless steel using EBSD and ab-initio calculations (Ruhr-Universität Bochum)

Dr.-Ing. M. Yao: κ -carbide in a high-Mn light-weight steel: precipitation, off-stoichiometry and deformation (RWTH Aachen)

2018

Dr.-Ing. F. Archie: Microstructural influence on micro-damage initiation in ferritic-martensitic DP-steels (RWTH Aachen)

Dr. rer. nat. Y.-H. Chen: A comprehensive in situ spectroscopic study of 2-mercaptobenzothiazole as a corrosion inhibitor for copper (Ruhr-Universität Bochum)

Dr.-Ing. W. S. Choi: Deformation mechanisms and the role of interfaces in face-centered cubic Fe-Mn-C micro-pillars (RWTH Aachen)

Dr. rer. nat. A. Frank: Synthesis and in-depth electron microscopic characterization of solvothermally grown copper indium sulfide thin films (RWTH Aachen)

Dr.-Ing. Q. Hu: A Contribution to Elucidate Interfacial Electric Double Layer Structures and Their Effects on Tribological Phenomena Using Force Microscopy (Ruhr-Universität Bochum)

Dr.-Ing. S. S. Katnagallu: On chemically sensitive atomic scale imaging (Ruhr-Universität Bochum), **with distinction "summa cum laude"**



Dr.-Ing. W. Krieger: Charakterisierung von Wasserstofffallen und deren Einfluss auf die Wasserstoffversprödung in ferritischen Stählen (Ruhr-Universität Bochum)

Dr.-Ing. A. Kwiatkowski da Silva: Phase nucleation through confined spinodal fluctuations at crystal defects in Fe–Mn alloys (RWTH, Aachen), **with distinction “summa cum laude”**

Dr. rer. nat. F. Niu: Investigation of interfacial water structure at Ge(100)/electrolyte interfaces by attenuated total reflection infrared spectroscopy (Ruhr-Universität Bochum)

Dr. rer. nat. J. S. Mondragón Ochoa: Preparation of Polyacrylic Thin Films on Iron by Controlled Radical Polymerization and their Delamination Behaviour (Ruhr-Universität Bochum)

Dr.-Ing. Z. Peng: Nano-scale investigation of the degradation mechanism of multilayer protective coating for precision glass molding (RWTH Aachen)

Dr. rer. nat. J. Rechmann: Modification of metal surface electronic properties by phenothiazine based SAMs (Ruhr-Universität Bochum)

Dr.-Ing. M. Schwan: Synthese und Eigenschaften flexibler Resorcin-Formaldehyd- und Kohlenstoffaerogele (RWTH Aachen)

Master Theses

2015 (not included in the Scientific Report 2013 - 2015)

Grabowski, M.: Implementation of atomic spin constraints in the density-functional theory package S/PHI/nX (Heinrich-Heine-Universität, Düsseldorf)

Lennartz, F.: Entwicklung eines automatisierten Profiling-Systems zur Dokumentation von Laufzeit und Speicherverbrauch für die Kristallplastizitätssoftware DAMASK (Fachhochschule Aachen)

Lu, L.: Characterization of the crack formation mechanism in Ni-based superalloy Inconel 738LC produced by Selective Laser Melting (SLM) (RWTH Aachen)

2016

Ksiazkiewicz, A.: Investigation of the surface chemistry of gelatine films on zinc (Ruhr-Universität Bochum)

Li, X.: Investigation of grain boundary fracture resistance in DP steel (RWTH Aachen)

Pander, M.: Depth-dependent vibrational spectroscopy at a water/electrode interface (Ruhr-Universität Bochum)

Qin, S.: Measurement of solidification characteristics of steel during Selective Laser Melting using high-speed pyrometry (RWTH Aachen)

Rashevski, D.: Development of an Interface to Couple the Düsseldorf Advanced Material Simulation Kit (DAMASK) with the Open Source Finite Element Library deal.II (RWTH Aachen)

Surendralal, S.: Automated Calculations for Charged Point Defects in Magnesium Oxide and Iron Oxides (Ruhr-Universität Bochum)

Wu, L.: Characterization of the microstructure and impurities of Al–Mg–Sc alloy produced by Laser Additive Manufacturing (RWTH Aachen)

2017

Ackers, M.: Recommissioning of a metal powder atomisation system and investigation of its suitability to produce powders for additive Manufacturing processes (Ruhr-Universität Bochum)

Mishra, A.: First principles calculations on field evaporation from metal surfaces (Ruhr-Universität Bochum)

Nastola, J.: Multi-scale modeling of hydrogen transport (Heinrich-Heine Universität, Düsseldorf)

Parra Moran, C.: Atomic scale analysis of grain boundary segregation in pearlitic steel (Escuela Superior Politécnica del Litoral, Guayaquil, Ecuador)

Qin, Y.: Effect of post-heat treatment on the microstructure and mechanical properties of SLM-produced IN738LC (RWTH Aachen)



2018

Baumgartner, L.-M.: Adsorption of coiled-coil peptides on substrates for ATR-IR spectroscopy (Heinrich-Heine-Universität, Düsseldorf)

Böckmann, M.: High-throughput thermodynamic modelling of precipitate formation employing empirical potentials (Heinrich-Heine-Universität, Düsseldorf)

Changizi, R.: Cathodoluminescence study of lanthanide-doped oxides (Heinrich Heine Universität, Düsseldorf)

Gänsler, T.: Synthesis approaches to Nb₃O₇(OH) nanostructures and new studies on their growth mechanism (LMU München)

Qin, S.: Measurement of solidification characteristics of steel during Selective Laser Melting using high-speed pyrometry (RWTH Aachen)

Shan, Y.: Investigation on the Influence of Hydrogen on Dislocation Formation during Nanoindentation in TWIP Steels (RWTH Aachen)

Shayanfar, N.: Ab-initio Thermodynamics of Interfaces of Metal-Heusler Composites (Ruhr-Universität Bochum)

Yang, Y.: 3-dimensional investigation of the crystallographic prior-austenite grain boundary characters in martensitic steels (RWTH Aachen)

Yilmaz, C.: Microstructural Investigations of Heavily Rolled Ni-9at.%W Sheets Designed as Substrate for Superconducting Layers (RWTH Aachen)

Bachelor Thesis

2018

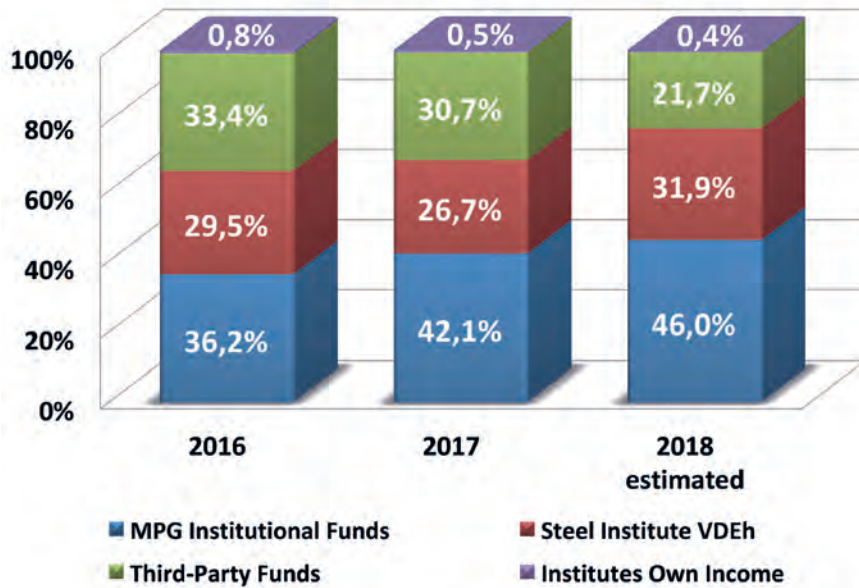
Bueno Villoro, R.: Effect of the processing route on the microstructure of Ag₁₈Sb₂₉Te₅₃ (AST) based thermoelectrics (Universitat Autònoma de Barcelona, Spain)



Budget of the Institute

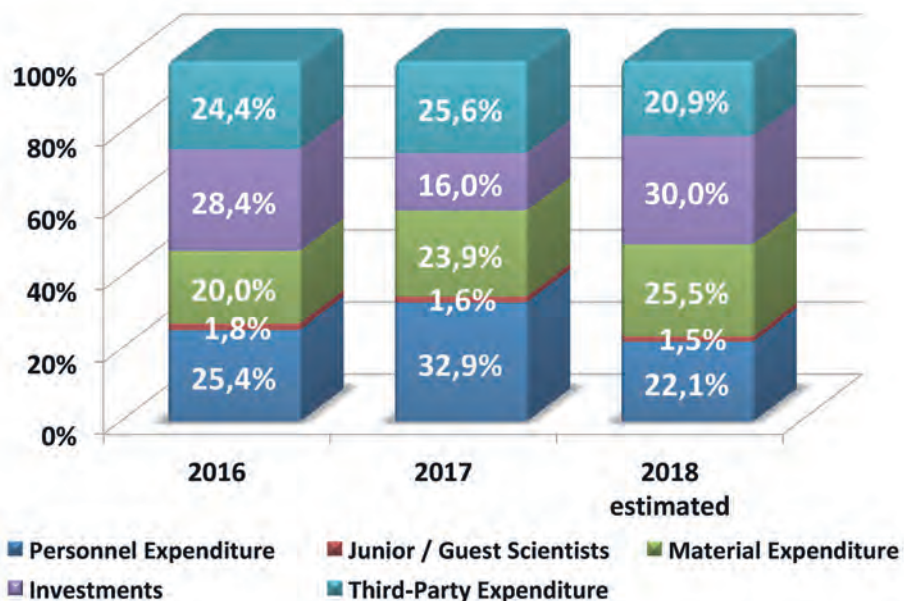
Revenue

(Percentual contributions to total revenue without appointment-related investment funds and general reconstruction of the buildings; year 2018 data estimated)



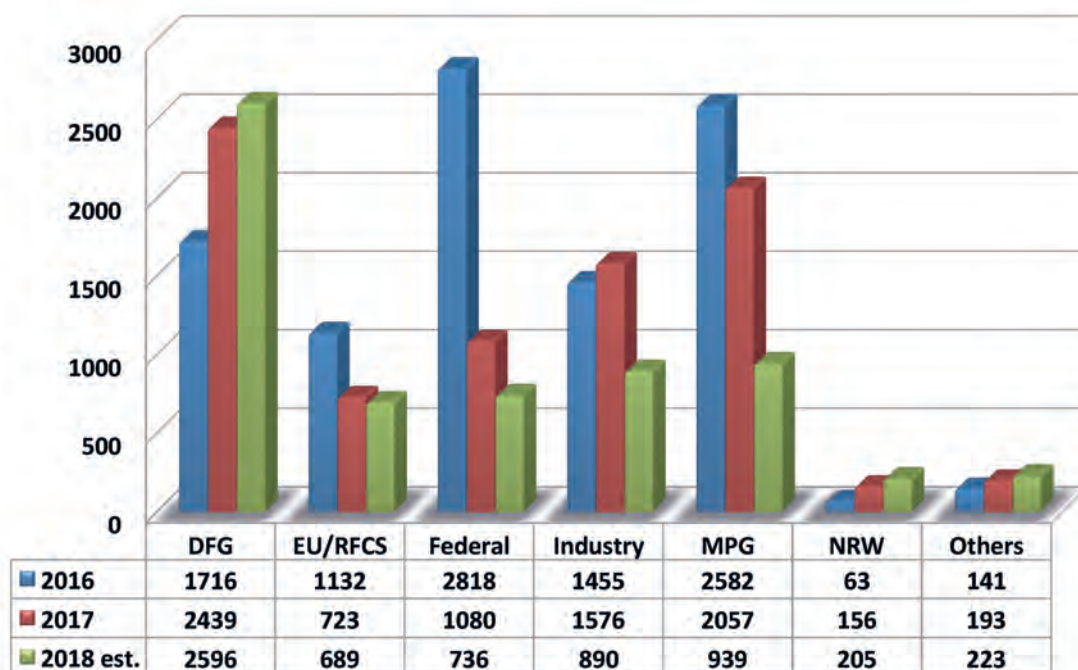
Expenditure

(Percentual distribution of total expenditure; investments include large-scale apparatus, electronic data processing, appointment-related investments, separate investment for basic equipment; year 2018 data estimated)



Third-Party Funds

(Contributions in 1,000 € to total revenue including personnel, material and investments, year 2018 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

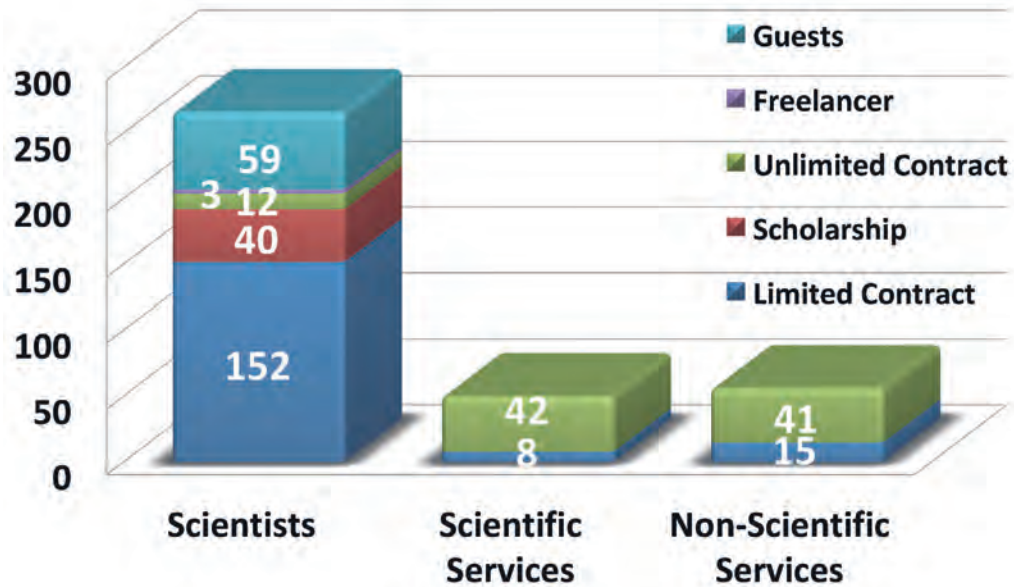
Industry incl. Christian Doppler Society and MaxNet
 MPG: Max Planck Society
 NRW: State of North Rhine-Westphalia
 Others: Diverse expenditure on material costs (e.g. Humboldt Foundation, Merkle Foundation)



Personnel Structure

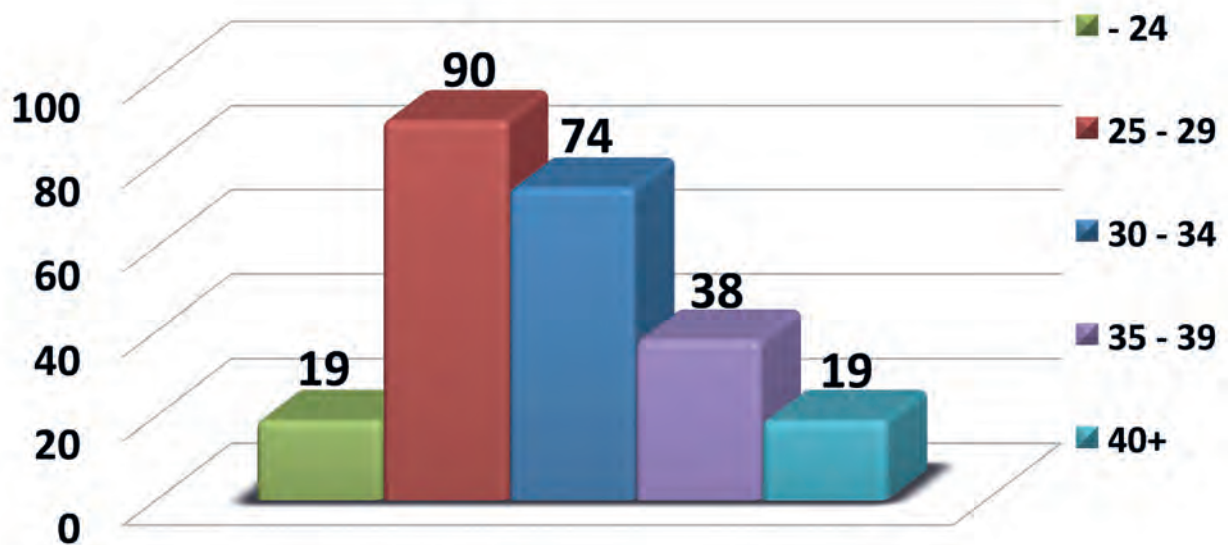
Number of Occupied Scientific / Non-Scientific Positions

(Absolute numbers, September 2018)



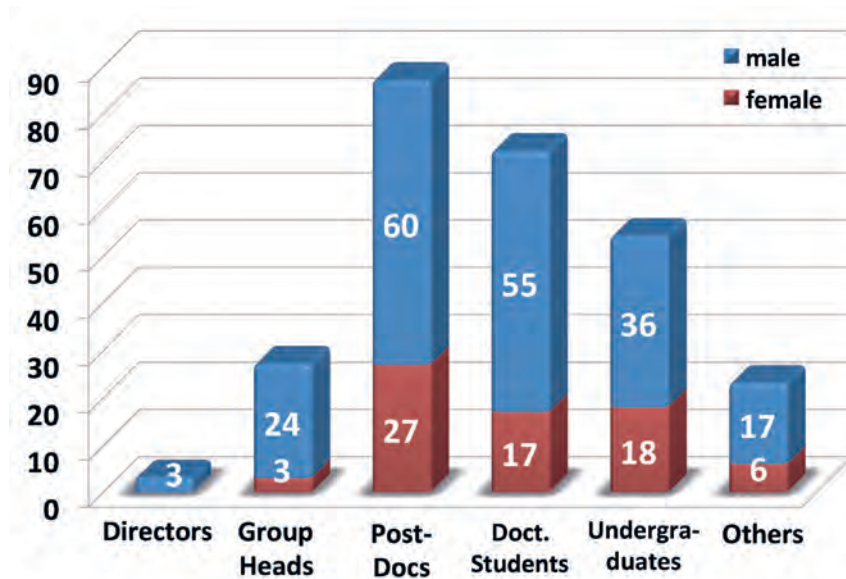
Age Distribution of Junior Scientists

(Absolute numbers, September 2018)



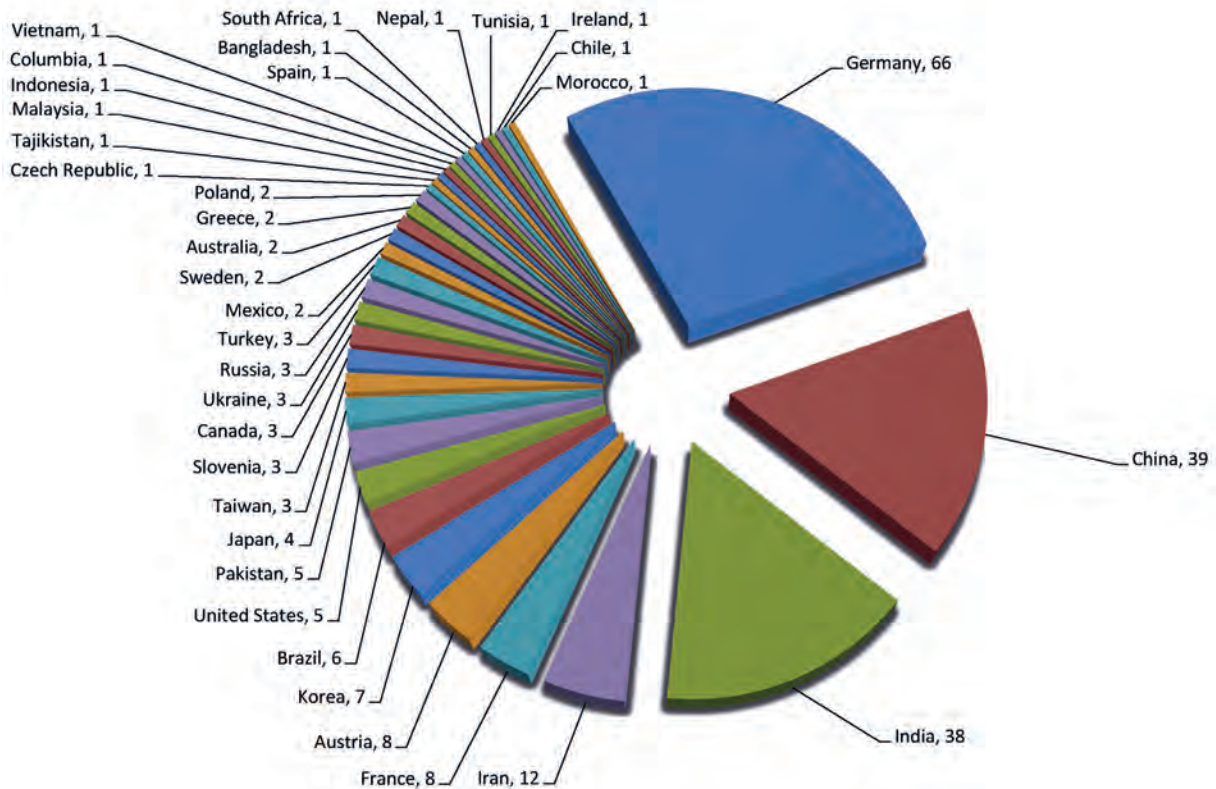
Gender Distribution of Scientists

(Absolute numbers, September 2018)



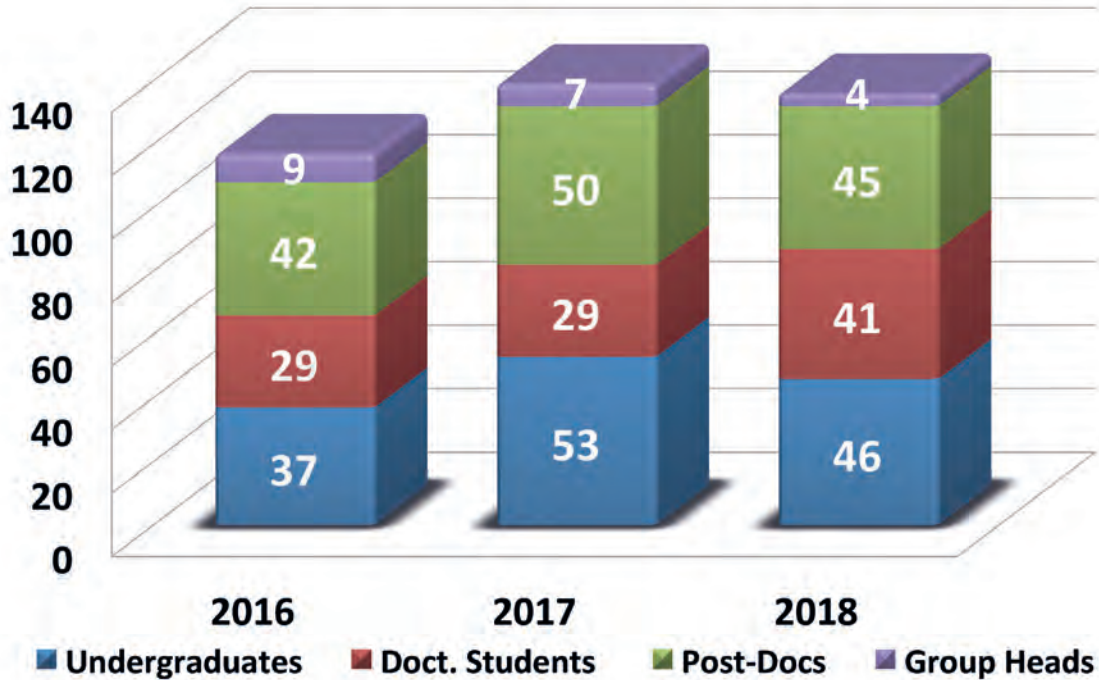
Scientists and their Home Countries

(Absolute numbers, September 2018)





Number of Junior Scientists (Absolute numbers, year 2018 data estimated)
Financed via Third-Party Funds



Not Financed via Third-Party Funds

