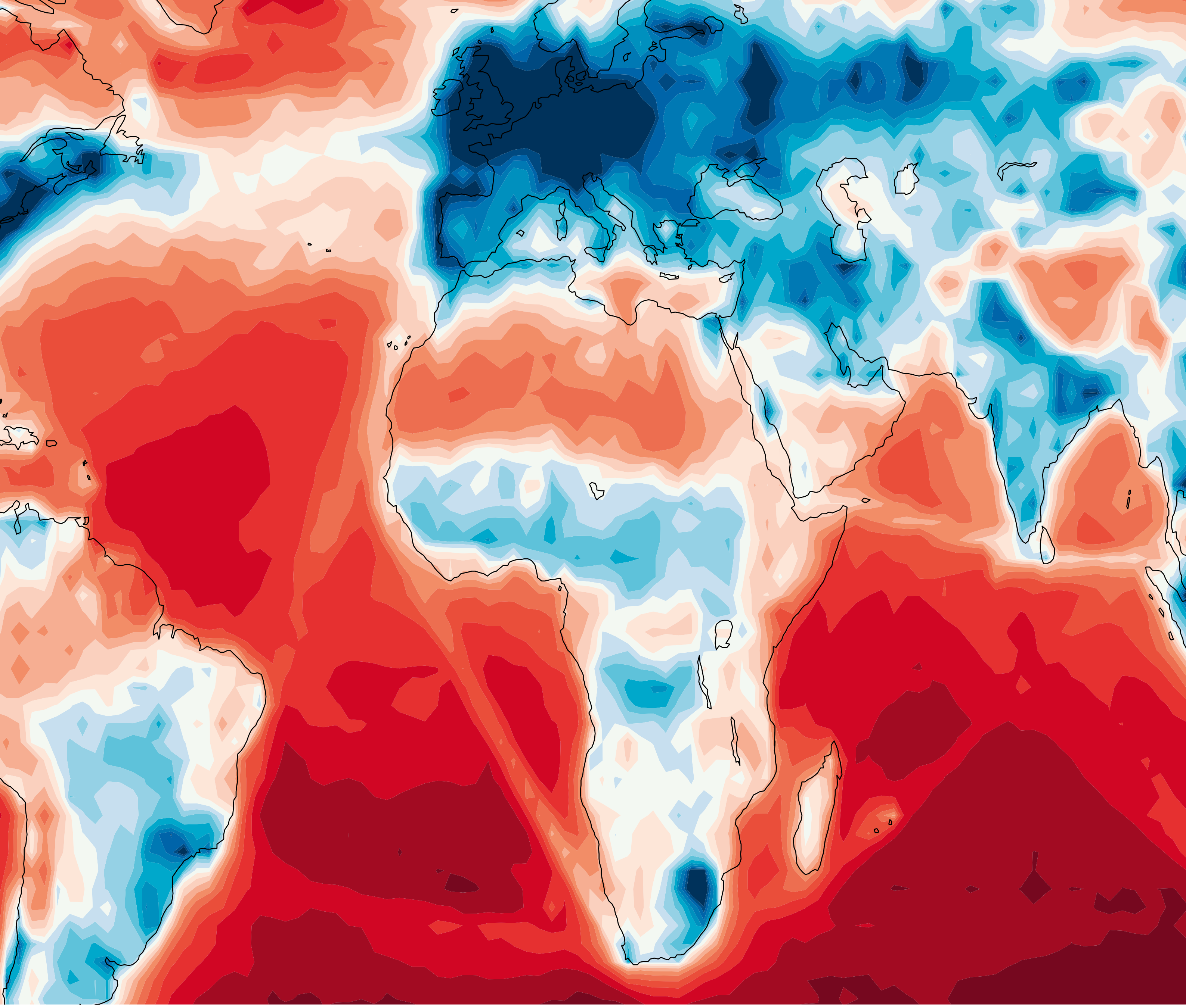


# SCIENTIFIC REPORT 2021 – 2023

## APPENDIX




MAX PLANCK INSTITUTE
FOR CHEMISTRY

# SCIENTIFIC REPORT 2021–2023 APPENDIX

**This document is an Appendix to the Scientific Report 2021–2023 of the Max Planck Institute for Chemistry and compiles non-public information for the Scientific Advisory Board.**

The Appendix relates to the reporting period 2021 to 2023 and is divided into the following sections:

1. Finances
2. Personnel distribution
3. Equal Opportunities
4. Memberships
5. Awards and Honors
6. Events
7. Scientific seminar talks
8. Scientific publications
9. Publication Impact Analyses

Figures and charts in the Finance, Personnel, and Equal Opportunities sections are exemplified by data from December 2022.

The Memberships section compiles the memberships of MPIC directors and scientific group leaders available at the editorial deadline in December 2023.

The Awards and Honors section details recognitions received by MPIC directors and scientific group leaders during the period 2021–2023.

The Events, Scientific Seminar Talks, and Scientific Publications sections encompass data from 2021 to 2023.

The Publication Impact Analyses documents were prepared externally by:

- Thomas Scheidsteger & Robin Haunschild, Max Planck Society, Information Retrieval Services (IVS-CPT), Stuttgart, Germany: Publication Output and Citation Impact - A bibliometric analysis of the MPI for Chemistry, Mainz, in the publication period 2012–2022
- Max Planck Digital Library (MPDL), Big Data Analytics, Munich: Publication Profile: Impact Max Planck Institute for Chemistry.

MAX PLANCK INSTITUTE
FOR CHEMISTRY

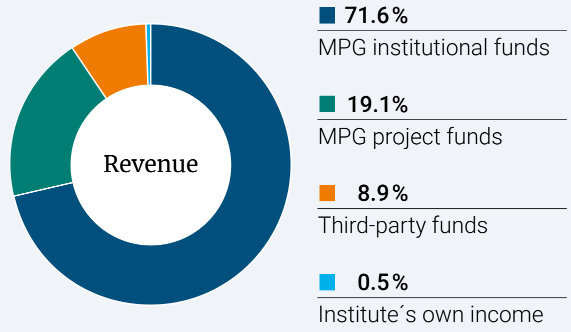
# 1 FINANCES

## REVENUES AND EXPENDITURES 2022

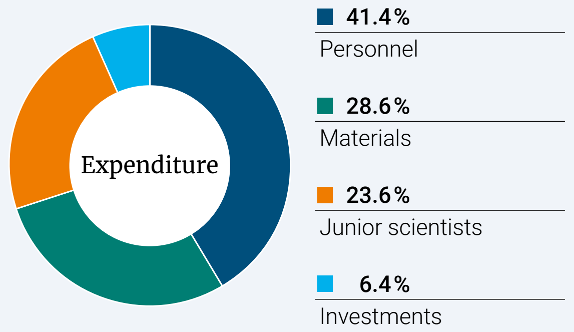
# 1. FINANCES: REVENUE AND EXPENDITURE 2022

**The annual budget of the Institute is approximately € 24 million. A major fraction derives from MPG institutional funds provided by federal and state governments. An overview of revenues and expenditures is given below.**

| Revenue | thousand EUR |
|---|---|
| MPG institutional funds | 17.454 |
| MPG project funds | 4.647 |
| Third-party funds | 2.161 |
| Institute´s own income | 123 |
| **Total income** | **24.385** |




| Expenditure | thousand EUR |
|---|---|
| Personnel | 10.097 |
| Materials | 6.972 |
| Junior scientists | 5.760 |
| Investments | 1.556 |
| **Total expenditure** | **24.385** |

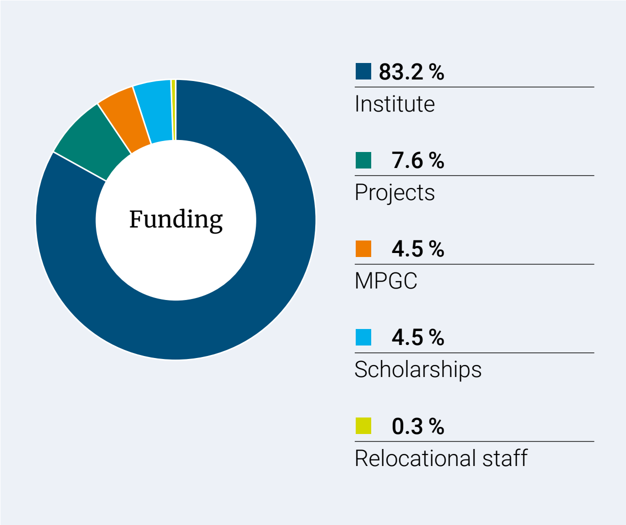


# 2 PERSONNEL DISTRIBUTION 2022

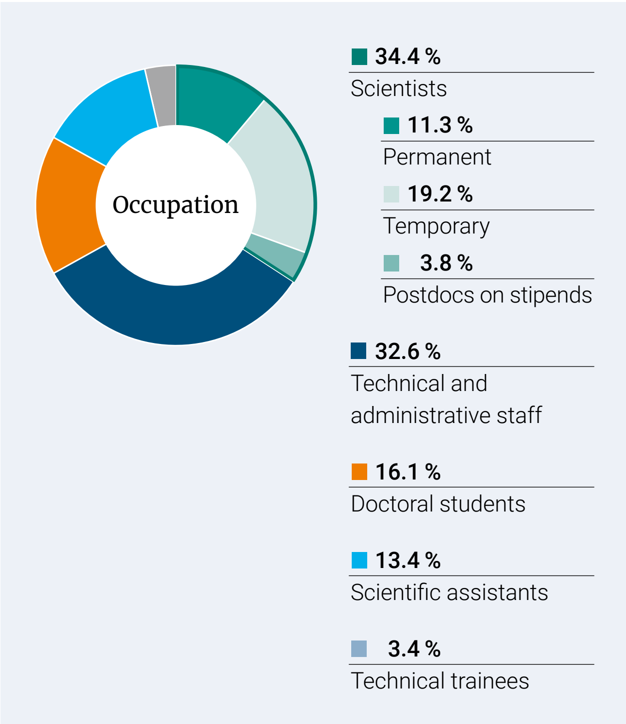
# 2. PERSONNEL DISTRIBUTION 2022

**In December 2022, a total of about 290 persons were employed at the Institute, among them 100 scientists, 47 PhD students and 10 technical trainees. 39.5 % of the staff were female, 60.5 % male. 242 staff members were paid from institutional funds, 22 scientists received payment from third-party project funding, 13 from scholarships and 13 by graduate schools.**

| Funding | persons |
|---|---|
| Institute | 242 |
| Projects | 22 |
| Max Planck Graduate Center | 13 |
| Scholarships | 13 |
| Relocational staff | 1 |
| **Total excl. guests** | **291** |

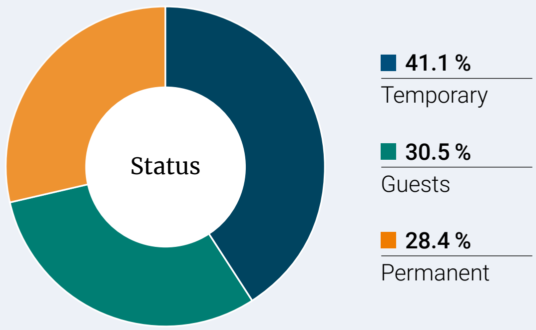



| Occupation | persons |
|---|---|
| Scientists | 100 |
| Permanent (incl. Directors) | 33 |
| Temporary (incl. Postdocs) | 56 |
| Postdocs on stipends | 11 |
| Technical and administrative staff | 95 |
| Doctoral students | 47 |
| Scientific assistants | 39 |
| Technical trainees | 10 |
| **Total excl. guests** | **291** |

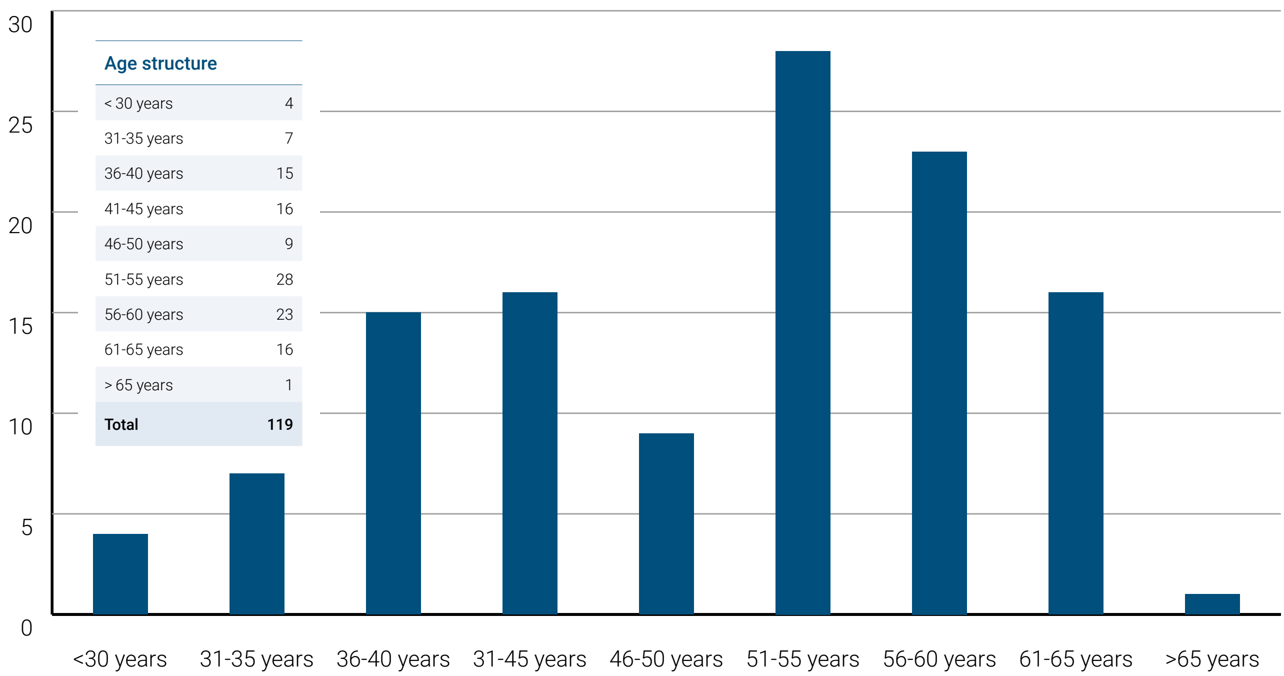


## Status of the MPIC staff including guests

| Status | persons |
|---|---|
| Temporary | 172 |
| Guests | 128 |
| Permanent | 119 |
| **Total** | **419** |




## Age distribution of the MPIC personnel with permanent contacts




| Age structure | |
|---|---|
| < 30 years | 4 |
| 31-35 years | 7 |
| 36-40 years | 15 |
| 41-45 years | 16 |
| 46-50 years | 9 |
| 51-55 years | 28 |
| 56-60 years | 23 |
| 61-65 years | 16 |
| > 65 years | 1 |
| **Total** | **119** |

MAX PLANCK INSTITUTE
FOR CHEMISTRY

# 3 EQUAL OPPORTUNITIES 2021 – 2023

# 3. EQUAL OPPORTUNITIES 2021–2023

**The Max Planck Institute for Chemistry is committed to supporting employees regardless of their gender, nationality, religion, disabilities, age, cultural background, or sexual identity. This commitment aligns with the Max Planck Society's strategic goal of providing equal opportunities for all employees, a goal further facilitated by the dedicated equal opportunities officers at the institute.**

The primary responsibility of the equal opportunities officers is to provide guidance to colleagues on matters related to career advancement, child care, and family support options, and to assist in eliminating discrimination. Since early summer 2023, we have introduced a parent-child room designed like a standard office but featuring a dedicated kids' corner equipped with toys and ample space, allowing individuals to work while also attending to their children's needs if necessary.

The equal opportunities officers are involved in all personnel, organizational and social measures relating to equality between genders, the reconciliation of family life and work as well as protection from sexual harassment at the workplace. Thus, they take part in job interviews and the institute meetings with the board of directors. The officers are well integrated into the everyday life at the institute by participating in discussions and meetings. They organize seminars and information events, also in cooperation with the neighboring Max Planck Institute for Polymer Research.

As per German law, the position of equal opportunities officers is exclusively open to women. To foster a more diverse and inclusive discussion on topics and challenges, particularly those faced by younger colleagues, we have established a gender equality team. This team comprises the equal opportunities officers along with two younger colleagues, one male and one female.

The equal opportunities plan is scheduled for revision in early 2024.

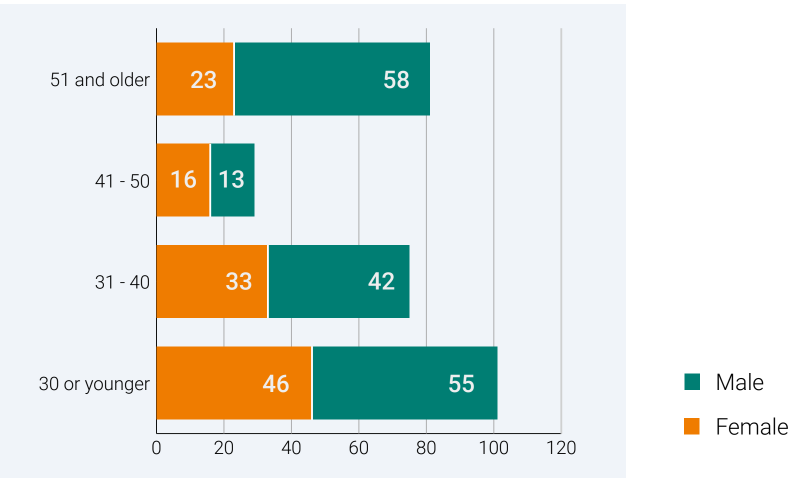
The equal opportunities page on the institute intranet provides information on gender equality topics through circulars, general information, and job offers.

Support options for families and female researchers are prominently advertised on the web pages of the institute (https://www.mpic.de/4161235/equal-opportunities).

Comprehensive information on the equal opportunity program of the Max Planck Society is available at https://www.mpg.de/central-gender-equality-officer.

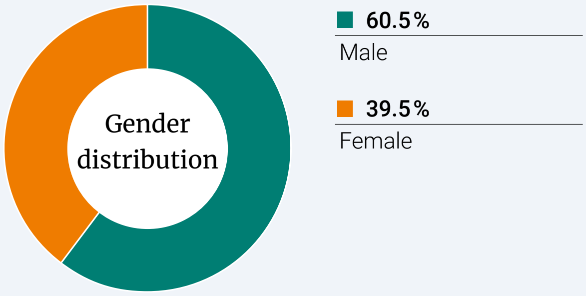
All figures and charts are exemplified by data from December 2022.

## Age structure of personnel (excl. guests)

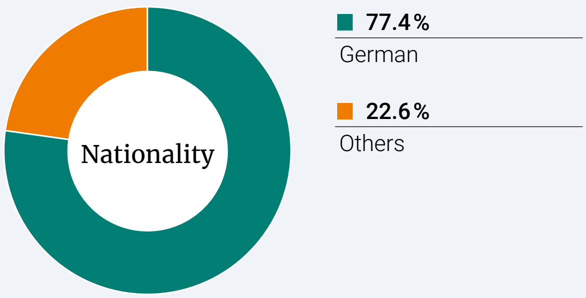


## Gender distribution and origin of the MPIC personnel

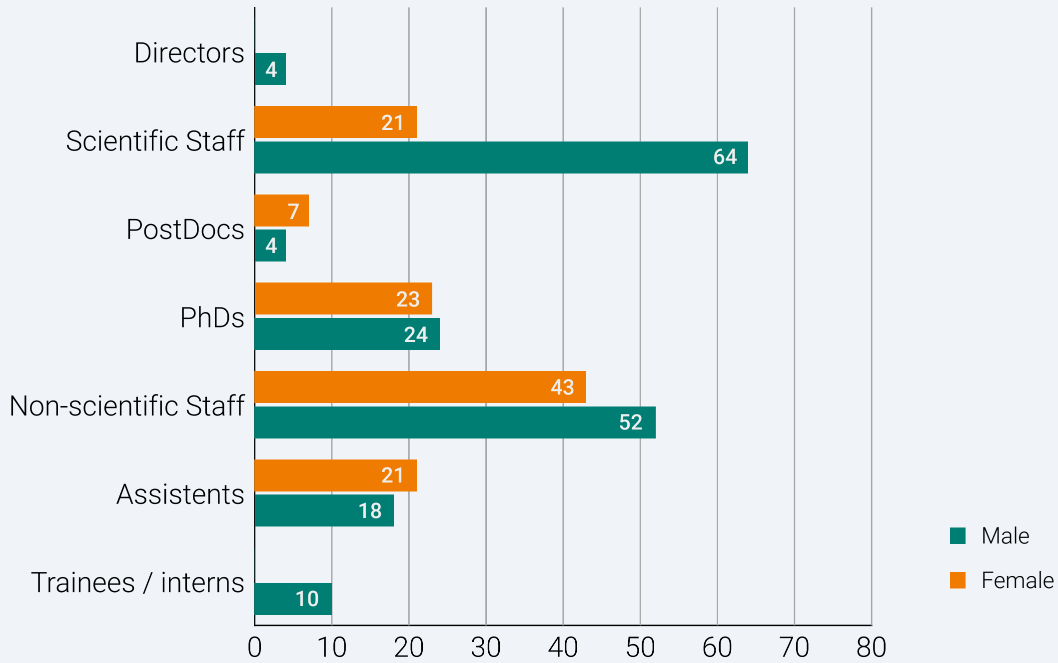
| Gender | persons |
|---|---|
| Male | 176 |
| Female | 115 |
| **Total excl. guests** | **291** |




| Nationality | persons |
|---|---|
| German | 224 |
| Others | 67 |
| **Total excl. guests** | **291** |

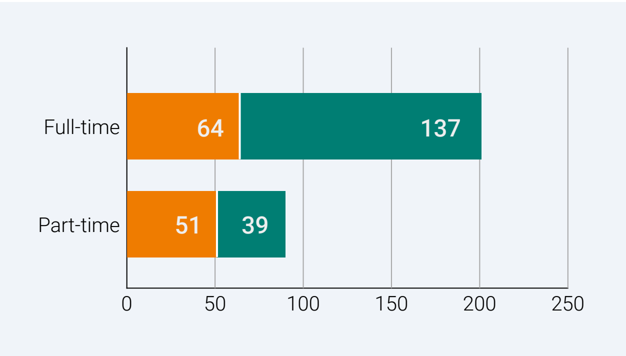



## Number of employees according to occupation

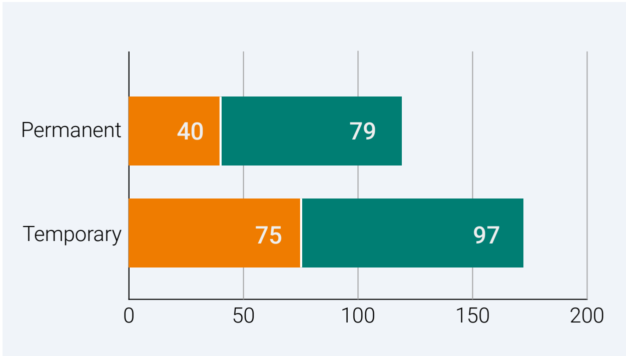


## Number of employees according to:

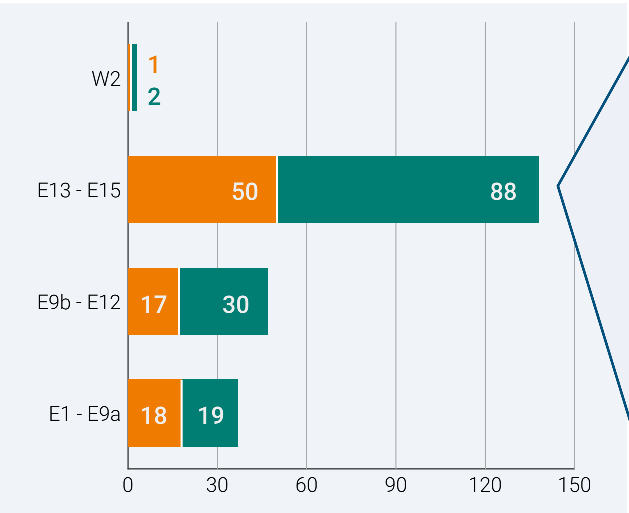
### • full - time or part - time positions



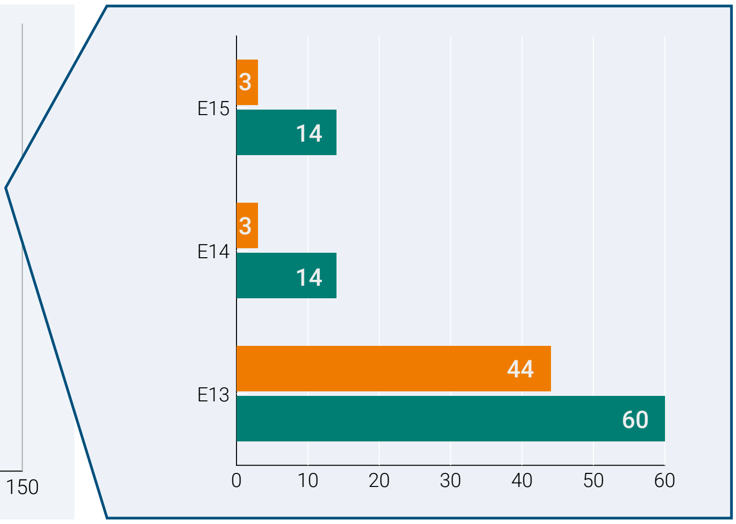

### • the contract type




### • payment




### • groups E 13 - E 15 only




Male
Female

## Salary scales at the MPIC

The salary scales at the Max Planck Society are based on the public sector pay scales in Germany, specifically the collective agreement for the public sector (TVöD) for federal and local government employees. Here's a breakdown of the subdivisions based on the pay groups:

According to the requirements of the respective position the subdivision is into

E 1 - E 4: semi-skilled and unskilled workers.
E 5 - E 9a: at least 2 or 3 years of vocational training.
E 9b - E 12: University of Applied Sciences or Bachelor's degree.
E 13 - E 15: academic university degree or Master's degree.

For postdocs in pay group E13, experience level 3, the monthly basic salary is stated to be around 4,911 euros gross per month in 2023 according to TVöD.

MAX PLANCK INSTITUTE
FOR CHEMISTRY

# 4 MEMBERSHIPS 2021–2023

# 4. MEMBERSHIPS 2021–2023

## ATMOSPHERIC CHEMISTRY DEPARTMENT – J. Lelieveld

### Jos Lelieveld (Director)

- American Geophysical Union (AGU)
- American Meteorological Society (AMS)
- Center for Clouds, Chemistry and Climate, Scripps Institution of Oceanography, University of California, San Diego (since 1992)
- Advisory Board of Tellus B (since 1996)
- Editorial Board of Journal of Atmospheric Chemistry (since 1996)
- Professor in Atmospheric Physics, University of Mainz (since 2002)
- Professor at the Cyprus Institute, Cyprus (since 2008)
- Spokesman for the International Max Planck Graduate School for Atmospheric Physics and Chemistry – now Paul Crutzen Graduate School (since 2002)
- Scientific-Technical Committee of the Executive Board, Karlsruhe Institute of Technology (KIT), Chair Advisory Board of the Atmosphere and Climate Program (2006–2019)
- Steering Committee Max Planck Graduate Center Mainz (since 2008)
- Editorial Board of Earth System Dynamics (since 2010)
- Selection and Evaluation Committee, Institute for Basic Science, South Korea (since 2013)
- German National Academy of Sciences – Leopoldina (since 2015)
- European Geosciences Union (EGU), life member (since 2015)
- International Silk Road Academy of Sciences and kick-off committee, China (since 2016)
- Royal Society of Chemistry, UK (since 2017)
- Guest editor of the Proceedings of the National academy of sciences (since 2019)
- Scientific Council of the National Observatory Athens (since 2019)
- Advisory Board of the Ruisdael Observatory, the Netherlands (since 2019)
- Advisory Board of the Panhellenic infrastructure for atmospheric composition and climate change (since 2019)

### John Crowley

- European Geosciences Union (EGU)
- International Union of Pure and Applied Chemistry (IUPAC): Task Group in Atmospheric Chemical Kinetic Data Evaluation

### Horst Fischer

- European Geosciences Union (EGU)
- International Union of Pure and Applied Chemistry (IUPAC): Task Group in Atmospheric Chemical Kinetic Data Evaluation

### Hartwig Harder

- Executive editor of Atmospheric Measurement Techniques (AMT)
- Section Representative of the Max Planck Institute for Chemistry, Mainz
- European Geosciences Union (EGU)
- American Geophysical Union (AGU)

### Andrea Pozzer

- Editor of Atmospheric Chemistry and Physics (ACP)
- European Geoscience Union (EGU)
- Editor of Elementa: Science of the Anthropocene
- Italian scientific habilitation (ASN) to full professor for section 04/A4 - Geophysics
- Italian scientific habilitation (ASN) to associate professor for section 02/C1 – Astrophysics and planetary physics
- Right to doctorate at the University of Mainz, Fachbereich 08, Meterology
- Adjunct Associate Professor at the Cyprus Institute since April 2022
- Member of the DKRZ (Deutsches Klimarechenzentrum) user group

## Jonathan Williams

- European Geosciences Union (EGU)
- American Geophysical Union (AGU)
- Fellow of the Royal Geophysical Society
- Adjunct Professor at the Cyprus Institute, Cyprus
- Editor of Atmospheric Chemistry and Physics (ACP)
- Editor for Environmental Chemistry, CSIRO publications
- Editor of Atmospheric Chemistry
- Faculty Member of the Max Planck Institute for Chemistry Graduate Center, Mainz

## CLIMATE GEOCHEMISTRY DEPARTMENT – G. H. Haug

### Gerald H. Haug (Director)

- German Academy of Science 'Leopoldina'
- Academia Europaea
- American Geophysical Union (AGU)
- Mainz Academy of Science and Literature

### Stephen J. G. Galer

- Meteoritical Society
- European Geosciences Union (EGU)
- American Geophysical Union (AGU)
- European Association of Geochemistry (EAG)

### Klaus Peter Jochum (Group leader until 2022)

- American Geophysical Union (AGU)
- International Association of Geoanalysts (IAG)
- Deutsche Mineralogische Gesellschaft
- Meteoritical Society
- Editorial Board of Geostandards and Geoanalytical Research
- Geochemical Society

### Alfredo Martinez-Garcia

- American Geophysical Union (AGU)
- Geochemical Society

### Bärbel Sarbas (Group leader until 2022)

- American Geophysical Union (AGU)
- International Association of Geoanalysts
- Deutsche Mineralogische Gesellschaft

### Ralf Schiebel

- Fellow of the Higher Education Academy (FHEA)
- Marine Micropaleontology, Editorial Board Member
- Journal of Foraminiferal Research, Cushman Foundation, Editorial Board Member
- Association of the Sciences of Limnology and Oceanography (ASLO)
- Deutsche Geologische Gesellschaft – Geologische Vereinigung (DGGV)

### Hubert Vonhof

- European Geosciences Union (EGU) Graduate Center, Mainz

# MULTIPHASE CHEMISTRY DEPARTMENT – U. Pöschl

## Ulrich Pöschl (Director)

- European Geosciences Union (EGU)
- Gesellschaft Deutscher Chemiker (GDCh)
- Founder and Chief Executive Editor of Atmospheric Chemistry and Physics (ACP)
- EGU Publications Committee
- Initiator and Co-chair of Open Access 2020 (OA2020)
- Membership Assembly of the Institute for Advanced Sustainability Studies (IASS)
- American Geophysical Union (AGU)
- EGU Governance Review Panel
- Advisory Board of ChemRxiv (American Chemical Society, Chineses Chemical Society, Chemical Society of Japan, German Chemical Society, Royal Society of Chemistry)
- Advisory Board of the GMPG Science History Research Program
- Steering Committee and Joint Board of the Max Planck Graduate Center with the Johannes Gutenberg University Mainz (MPGC)
- Speaker of the Max Planck Graduate Center with the Johannes Gutenberg University Mainz (MPGC)
- Consortium Council, Environmental Research Station Schneefernerhaus (2023)
- University Council, Augsburg University (2023)

## Thomas Berkemeier

- American Geophysical Union (AGU)
- Mainz Institute of Multiscale Modelling (M3ODEL) Steering Committee Member
- MPGC Junior Faculty Member (Spokesperson)
- Editorial Board member of Atmospheric Chemistry and Physics (ACP)
- International Aerosol Modelling Algorithms Conference Planning Committee Member
- MPGC Focus Group Interdisciplinary Numerical Modelling Techniques (Spokesperson)

## Janine Fröhlich

- European Geosciences Union (EGU)
- Mainz Program for Chemical Allergology (MPCA)
- Mainz Bioaerosol Laboratory (MBAL)

## Gerhard Lammel

- European Chemical Society (EuCheMS) Division of Chemistry and the Environment, Delegate
- International Union of Pure and Applied Chemistry (IUPAC) Division VI Chemistry and the Environment, National Representative
- American Geophysical Union (AGU)
- Member of Faculty (Privatdozent), Faculty of Chemistry, Pharmaceutical Sciences and Geosciences, University of Mainz
- Member of Faculty (Full Professor), Faculty of Sciences, Masaryk University, Brno, Czech Republic
- Member of Faculty, Max Planck Graduate Center (MPGC), Mainz
- Associate editor of Environmental Science and Pollution Research, Springer Nature
- German Chemical Society (GDCh)
- ProcessNet/GDCh/KRdL-Gemeinschaftsausschuss Feinstäube
- ProcessNet/GDCh/Bunsengesellschaft-Geimeinschaftsausschuss Chemie-Luftqualität-Klima
- UNEP Stockholm Convention, Global Monitoring Plan, Member of Central and Eastern Europe Regional Organization Group

## Kurt Lucas

- Mainz Program for Chemical Allergology (MPCA)
- European Academy for Molecular Hydrogen Research in Biomedicine, Member of the Board of Directors
- Laboratory of Inflammation & Microscopy (LIM)
- Mainz Bioaerosol Laboratory (MBAL)

## Mira Pöhlker

- Aerosol, Cloud, Precipitation, and Climate Working Group (ACPC)

## Christopher Pöhlker

- ATTO Scientific Steering Committee
- German Chemical Society (GDCh)

## Hang Su (Group leader until 08/23)

- American Association for the Advancement of Science (AAAS)
- American Geophysical Union (AGU)
- European Geoscience Union (EGU)
- Gesellschaft für Aerosolforschung (Gaef)

## PARTICLE CHEMISTRY DEPARTMENT – S. Borrmann

### Stephan Borrmann (Director)

- Deutsche Meteorologische Gesellschaft (DMG)
- Deutsche Physikalische Gesellschaft (DPG)
- International Committee for Clouds and Precipitation (ICCP)
- European Geosciences Union (EGU)
- Member of the Board of Directors of the Görres Gesellschaft at the Institute of Interdisciplinary Research between Science, Philosophy and Theology
- Member of the Board of Trustees at Academia Sinica of the National University of Taiwan
- Visiting Professor at the University of Manchester (since 2022)

### Frank Drewnick

- Deutsche Physikalische Gesellschaft (DPG)

### Peter Hoppe

- Meteoritical Society (Fellow since 2002)
- Swiss Physical Society (SPG)
- European Association of Geochemistry (EAG)
- German Physical Society (DPG)

### Johannes Schneider

- Deutsche Gesellschaft für Aerosolforschung (GAeF)
- European Geosciences Union (EGU)
- Committee on Nucleation and Atmospheric Aerosols (CNAA)
- Deutsche Physikalische Gesellschaft (DPG)

### Miklós Szakáll

- Scientific Section of Earth Sciences (Committee on Meteorology) of the Hungarian Academy of Sciences
- European Geosciences Union (EGU)
- Hungarian Meteorological Society

## INDEPENDENT RESEARCH GROUPS

### Yafang Cheng

- Member of Academia Europaea (MAE)
- Fellow of American Geophysical Union (AGU); Member of AGU
- Honor committee member for Atmospheric Sciences Ascent Award of AGU (since 2022)
- Member of European Geosciences Union (EGU)
- Liaison for Atmospheric Sciences Division of EGU (Since 2013)
- Editor-in-chief of the Journal of Geophysical Research: Atmosphere (since 2023)
- Senior Editor of Atmospheric Chemistry and Physics (ACP) overseeing the subject area of aerosols (2020–2022); Co-editor of ACP (since 2013)
- Member of American Association for the Advancement of Science (AAAS)
- Member of American Meteorological Society (AMS)
- Member of American Chemical Society (ACS)
- Member of Gesellschaft für Aerosolforschung (Gaef)
- Committee member of CNAA (The committee on Nucleation & Atmospheric Aerosols, 2023–2025)
- Guest professor at the Peking University (since 2023)
- Distinguished guest professor at the University of Science and Technology of China (USTC, 2021–2024)

### Mikhail Eremets

- Editorial Board, High Pressure Research Journal, Taylor and Francis
- Advisor committees: CIMTEC congress, Italy
- Member of Commission on Crystallography of Materials of the International Union of Crystallography
- American Physical Society (APS)
- American Association for the Advancement of Science (AAAS)
- Sigma Xi the Scientific Research Society
- American Geophysical Union (AGU)
- Max Planck Graduate Centre (MPGC)

### Tina Lüdecke

- American Association of Biological Anthropologists (AABA)
- East African Association of Paleoanthropology and Paleoecology (EAAPP)
- European Society of the study of Human Evolution (ESHE)
- Frankfurter Geographische Gesellschaft
- Max Planck Graduate Center (MPGC)

### Thomas Wagner

- European Geosciences Union (EGU)
- Chief Executive Editor of the Journal of Atmospheric Measurement Techniques (AMT)
- Quality working group for the Sentinel 5 precursor satellite
- Science Advisory Group of the Korean GEMS satellite (Geostationary Environment Monitoring Spectrometer)
- Science Advisory Group for the satellite instruments GOME and GOME-2A/B

## FORMER DIRECTORS

### Meinrat O. Andreae
**(Director of the Biogeochemistry Dept. until 2017)**

- European Geosciences Union (EGU)
- American Chemical Society
- American Geophysical Union (AGU)
- American Association for the Advancement of Science (AAAS)
- The Geochemical Society
- Member, SCIENCE Board of Reviewing Editors
- Brazilian Academy of Science
- American Academy of Arts and Science
- Fellow of the American Geophysical Union (since 2014)
- Advisory Board Atmospheric Chemistry and Physics
- Scientific Steering Committee for the Large-Scale Biosphere/Atmosphere Project in Amazonia (LBA)
- Scientific Steering Committee for the German HALO Research Aircraft
- Past Chair, Core Project "Integrated Land-Ecosystem Atmospheric Processes Study (ILEAPS)" of IGBP II
- Vice-Chairman, German National Committee for Global Change Research
- Advisory Board of the International Institute for Applied Systems Analysis (IIASA)

### Albrecht W. Hofmann
**(Director of the Geochemistry Dept. until 2007)**

- American Geophysical Union (AGU), member
- Geological Society of America (GSA)
- Geochemical Society
- European Association of Geochemistry
- Deutsche Mineralogische Gesellschaft
- Geologische Vereinigung

# 5 SCIENTIFIC AWARDS AND HONORS 2021 – 2023

# 5. SCIENTIFIC AWARDS AND HONORS 2021–2023

## DIRECTORS

**Jos Lelieveld**
- Research.com Environmental Sciences in Germany Leader Award 2022, 2023
- Distinguished lecturer at the King Abdullah University of Science and Technology, 2023
- Highly Cited Researcher in the field of Cross-Field (top 0.1%), Web of Science & Clarivate, 2021, 2022, 2023
- Cardiovascular Research High Impact Paper Award (European Society of Cardiology ESC), 2021

**Ulrich Pöschl**
- Union Fellow of the American Geophysical Union (AGU), 2023
- Highly Cited Researcher in the field of Geosciences (top 0.1%), Web of Science & Clarivate, 2021, 2022, 2023

**Gerald H. Haug**
- Foreign Member of the Royal Society, ForMemRS, 2023
- Honorary Doctorate University of Heidelberg, Dr. h.c., 2023
- Fellow of the American Geophysical Union (AGU), 2022

## FORMER DIRECTORS

**Meinrat O. Andreae**
(Director of the Biogeochemistry Dept. until 2017)
- Highly Cited Researcher in the field of Gesciences (top 0.1%), Web of Science & Clarivate, 2021, 2022, 2023

**Paul J. Crutzen**
(Director of the Atmospheric Chemistry Dept. until 2000)
- Posthum: Future of Life Award 2022, Future of Life Institute

## SCIENTIFIC GROUP LEADERS

**Yafang Cheng**
(Minerva Group Leader Position since 2014)
- Fellow of American Geophysical Union (AGU), 2022
- Member of Academia Europaea, 2022
- Joanne Simpson Medal, American Geophysical Union (AGU), 2022
- Science Breakthroughs of the Year 2021 in Physical Scienc
- Highly Cited Researcher (top 0.1%), Web of Science & Clarivate, 2021, 2022

**Frank Drewnick**
(Group leader of the Particle Chemistry Dept.)
- AS&T Outstanding Reviewer Award, American Association for Aerosol Research, 2021

**Mikhail Eremets**
(Leader of the High pressure chemistry and physics group)
- The Bragg Lecture at University College London, 2023
- Bernd T. Matthias Prize for superconducting materials, 2022
- Bodo-von-Borries Special lecture, 2022

**Horst Fischer**
(Group leader of the Atmospheric Chemistry Dept.)
- Outstanding Reviewer, American Geophysical Union (AGU), 2021

**Johann Georg Goldammer**
(Former group leader of the Biogeochemistry Dept. until 2017)
- Honorary Doctorate of the Aristotle University of Thessaloniki, 2022
- "Bintang Jasa Utama Republic of Indonesia" Order of Merit, 2021

**Klaus Peter Jochum**
(Group leader of the Climate Geochemistry Dept. until 2022)
- Honorary Fellowship of the International Association of Geoanalysts (IAG), 2021

**Mira Pöhlker**
(Team leader of the Multiphase Chemistry Dept. until 2021)
- Minerva Fast track position

**Jonathan Williams**
(Group leader of the Atmospheric Chemistry Dept.)
- ERC Grant "Digitising Smell: From Natural Statistics of Olfactory Perceptual Space to Digital Transmission of Odors", 2023
- IG-Nobel Prize for Chemistry, 2021

## FURTHER SCIENTISTS

**Simone Andersen**
(Member of the Crowley Research Group)
- Humboldt Research Fellowship, 2023

**Anna Backes**
(Member of the Berkemeier Research Group)
- Otto Hahn Medal, 2021

**Chaoyang Xue**
(Member of the Minerva research group of Yafang Cheng)
- Humboldt Research Fellowship, 2023-2025

**Renyi Zhang**
(Visitor of the Minerva research group of Yafang Cheng)
- Humboldt Research Award, 2023

**Guangjie Zheng**
(Member of the Minerva research group of Yafang Cheng)
- Division Outstanding Early Career Scientist Award for Atmospheric Sciences, European Geosciences Union, 2023
- James J. Morgan Award Early Career Award: Honorable Mention, American Chemical Society, 2022

2021 the International Association of Geoanalysts (IAG) has awarded Dr. Klaus Peter Jochum an Honorary Fellowship for his years of service and numerous outstanding contributions to geoanalytical research.

# 6 EVENTS 2021 – 2023

# 6. EVENTS 2021–2023

**Several external and internal events occurred at the institute between 2021 and 2023. Owing to the Covid-19 pandemic, only a limited number of in-person meetings and workshops were conducted in 2021.**

The pages below categorize both internal and external events into
- scientific meetings, such as conferences and workshops
- events doctoral students (Paul Crutzen Graduate School, Max Planck Graduate Center) and postdocs,
- institute visits and outreach activities,
- trainings on equal opportunities*,
- workshops, courses and seminars on mental and physical health*,
- work safety events*, and
- further gatherings.

MPIC Scientific talks (Wednesday Seminar) are listed separately.

* The Max Planck Society provides a range of courses, webinars, and training programs to all employees for career development, further education, health, and safety (see also https://max.mpg.de/Career/Documents/Talent_Companion.pdf). Please note that these events are not listed.

## Scientific meetings

### 2021

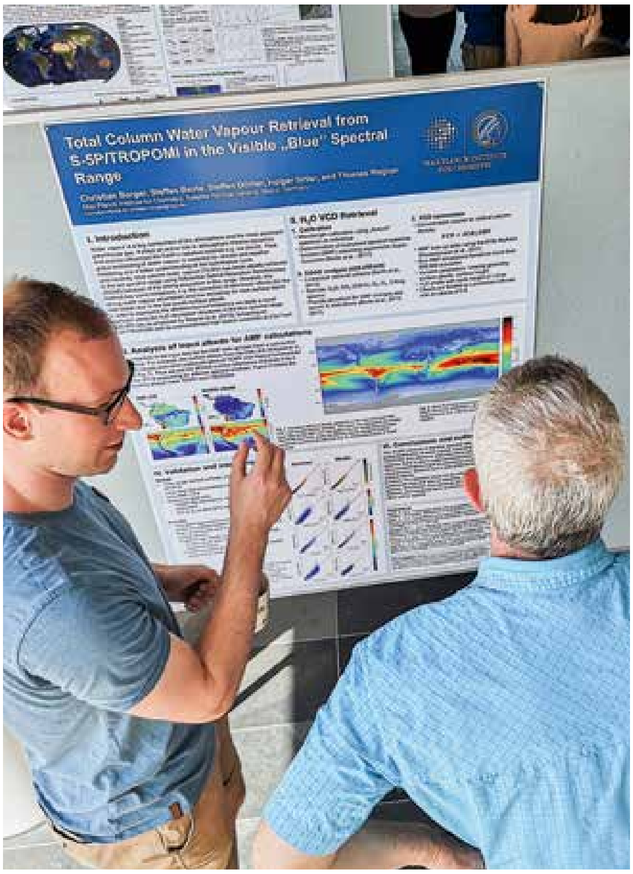
- **23–15 February**: Scientific Advisory Board Meeting, online
- **8–10 June**: ESRP meeting, online
- **17 June**: Posterday, online (see picture)
- **29 June**: Research Meeting with the University RheinMain (HSRM), online
- **5 July**: Full day course on air pollution and health within the Q+ study program of the JGU, online
- **28 September**: Celebration of awarding the honorary IAG Fellowship to K. P. Jochum, hybrid
- **11–15 October**: ATTO Meetings, hybrid
- **16 November**: Research Meeting Orbitrap for Isotopes, Lüdecke, online

### 2022

- **17 January**: Research Meeting S/Y Eugen Seibold
- **8 February**: BLUESKY Meeting – online
- **25–27 April**: ATTO meetings
- **30–31 May**: ESRP meeting Jena, Germany
- **19–20 September**: Celebration 20 years of OA journal: Atmospheric Chemistry and Physics
- **12–13 December**: Workshop SIBER (Stable Isotope Bayes-ian Ellipses in R)

### 2023

- **2 May**: Workshop with students from Hochschule Bonn-Rhe-in-Sieg
- **9–11 May**: 11th Annual EMAC Symposium
- **30 May–1 June**: CAFE-Brazil Workshop
- **5 June**: Meeting on Horizon EU call for non-communicable diseases
- **13–15 June**: ESRP Meeting, Göttingen, Germany
- **28 June**: Posterday
- **27–29 September**: Kick off Meeting Human Frontier Science Program, T. Lüdecke




## Events for doctoral students (Paul Crutzen Graduate School, Max Planck Graduate Center), and postdocs

Under the roof of the **Planck Academy**, the Max Planck Society offers its scientific members and staff opportunities for further education and personal career development. All MPS employees can choose from target-group-specific opportunities for further training and personal career development. The Planck Academy focuses on topics that strengthen affiliation with the MPG, convey its values, and enable closer networking among each other.

The career services for employees are structured into offers for Scientific Leaders, Group Leaders, Postdocs (see screenshot from intranet page), Doctoral Students, Science management & administration. A combination of suitable formats for exchange, community building, knowledge transfer and support through a wide variety of career phases within MPG are available.

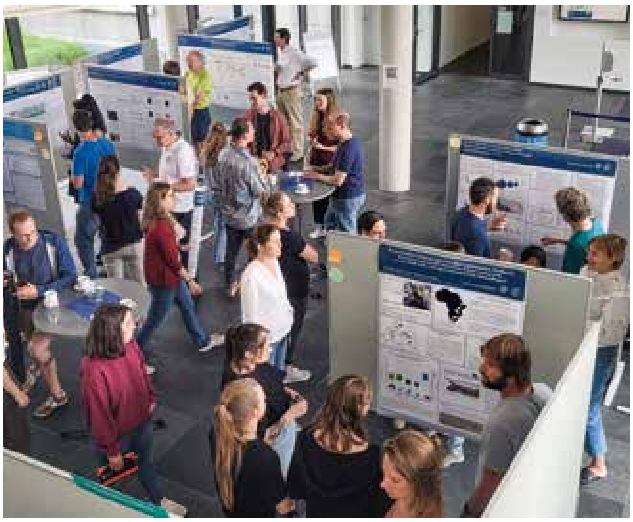
Additionally, the following courses take/took place at the institute.

### Recurring

- Lecture Cycle of the Max Planck Graduate Center (MPGC), each Wednesday during term
- English for PhD students for the Natural Sciences, permanently

### 2021

- **9 February**: Excellence@WORK - Gutenberg Alumni Talks in Natural Sciences
- **28–29 October**: Thesis defense training
- **9 November**: Social media in the professional context
- **19 November**: Improved reading
- **3 December**: Self-care for PhD students
- **9–10 December**: Thesis defense training



### 2022

- **25 January**:PhD General Meeting
- **8 February**: Media training
- **8 June**: MPGC Retreat
- **27 June**: MPIC+MPIP Posterday
- **28–29 July**: Thesis defense training
- **28 September**: Good Scientific Practice
- **29–30 September**: Workshop Land-atmosphere interactions at the ATTO-Campina sites
- **7 October**: Paul Crutzen Graduate School Days
- **31 October**: PhD General Meeting
- **Lecture series**: Atmospheric Chemistry, winter term 2022/23, Lammel

### 2023

- **27+28 February**: MPGC Evaluation
- **27 July**: MPIC+MPIP Posterday
- **9 October**: MPGC Retreat
- **5 December**: PhD General Meeting
- **Summer term PhD Lecture Series** – Lectures from Scientists for Scientists
- **Lecture Series**: Atmospheric Chemistry, G. Lammel; summer term

# Institute visits and outreach activities

## 2021

Due to Covid-19 restrictions there were no in person visits at the institute

- **11+12 September**: Mainz Science fair – online

## 2022

- **2 July**: Family Day together with the Rabanus Maurus Gymnasium (a secondary school)
- **6 July**: Group visit of Young Pakistani Scientists
- **23 July**: Group visit of the Rotary International Youth Organization
- **26 July**: Group visit of the International Summer School of the Faculty of Chemistry, Pharmaceutical Sciences, Geography and Geoscience of the JGU Mainz
- **28 July**: Visit of the Rhineland-Palatinate Minister of Science Clemens Hoch
- **20 December**: Visit of a delegation of the Rhineland-Palatinate consumer advise center

## 2023

- **27 February**: Scientific delegation from ACCA21, MOST, China
- **7 March**: Visit of the MPG President Prof Patrick Cramer
- **8 March**: Delegation of the Australian National University, Canberra, Australia
- **15 March**: Visit of a student group from the Wageningen University, The Netherlands
- **27 April**: Girl´s Day
- **23 June**: Max Planck Day, Göttingen, Germany
- **9 July**: Open Day at the MPIC
- **17 August**: Scientific Delegation from South Korea; M. Eremets
- **22 August**: Group visit from Columbia
- **9+10 September**: Mainz Science fair
- **25–28 September**: Scientific Delegation from the Jinan University, China
- **14 November**: Student group of the Kurfürstliches Gymnasiums Mainz
- **22 November**: Scientific Delegation from South Korea; MOU with MPIC, T. Wagner
- **14 December**: Group visit of the ECOS company

## Trainings on equal opportunities

The Max Planck Society offers provides offers for female scientists with the Minerva-FemmeNet and the Elisabeth-Schiemann-Kolleg. Minerva-FemmeNet is a network for female scientists in the Max Planck Society. Its aim is to pass on the expert knowledge of experienced female scientists – including former institute members – by mentoring junior female scientists.

Within the Elisabeth-Schiemann-Kolleg scientific members of the Max Planck Society foster the careers of excellent female scientists after their postdoc phase, helping them to succeed on their way to a possible appointment as a University Chair or a director at a Max Planck Institute.

Further, the Max Planck Society takes part in the MuT - Mentoring und Training. The MuT mentoring program is female addressing lecturers, junior professors, Habilitandinnen, postdocs and doctoral students at universities and universities of applied sciences in Baden-Württemberg

The MPG LeadNet is a bottom-up initiative and network bringing together senior scientists, research associates, project and group leaders of the Max Planck Society. LeadNet provides a forum for common scientific and organizational issues and promotes interactions among research groups within the MPG.

For more information, please refer to www.mpg.de/8332885/gender-equal-career-development.

Additionally, the following courses take/took place at the institute.

### 2021

- **15 September**: Gender equality in everyday life at the institute / rights and obligations in gender equality issues, online

### 2022

- **5 October – 2 November**: "Survey on work and management culture and on mental stress"

### 2023

- **7 February**: Mentoring program Minerva-FemmeNet and other MPG initiatives
- **12 September**: mandatory training on dialing with sexualized discrimination, harassment and violence
- **12 December**: Diversity, Equity & Inclusion: Just a trend or genuine benefit?


## Workshops, courses and seminars on mental and physical health

In addition to various courses and events partially organized by a health insurance company and listed below, the Max Planck Society provides the Employee and Manager Assistance Program (EMAP). This service offers support in addressing professional or personal challenges that may impact well-being at work. Immediate counseling is available through pme Family Service, accessible by phone, online, or in person. The consultation is free of charge, and it extends to include relatives living in the household.

Furthermore, the institute actively supports events such as running and biking, and provides each staff member with a free influenza vaccination each year.

In the summer of 2021, the institute provided staff members with two free COVID-19 vaccination opportunities.

### 2021

- **8 March**: Webinar "What is healthy nutrition anyway? A scientific search for traces"
- **25–28 May 2021**: Digital Health Week – de+en
- **Sober Curious** - a health-conscious lifestyle without alcohol
- **19 July: Webinar** "Occupational health management and the role of drinking in the workplace"
- **29 September**: interactive Workshop "Quick relaxation"
- **4–8 October 2021**: Max Planck Mental Health Awareness Week – online
- **27 October**: interactive Workshop "BrainFit- stay concentrated and fit"
- **30 November**: interactive Workshop "Winter blues – no thanks!"
- **6–10 December 2021**: Health Week, de+en – online + in person
- **Seminar**: How to protect yourself against stress & burnout
- **Yoga trial course**
- **Stress Type Identification**

### 2022

- various **Yoga and gymnastics courses**
- **19 January**: interactive Workshop "Loslegen und dranbleiben" (Get started and keep at it)
- **14–18 February**: Digital Health Week, de+en
- **7 March 2022**: National Day of Healthy Food &Cooking, de+en
- **11 May**: interactive Workshop "You are what you eat!"
- **22 May**: Post-Covid - Wie wir wieder zurück ins (Arbeits-) Leben finden (How we find our way back into (working) life), Fürstenberg institute
- **15 June**: interactive Workshop: „Positive Mindset"
- **7 und 8 July**: Planck Academy Days on sustainable leadership and resilience, de+en
- **13 July**: interactive Workshop „Full Body Mobility"
- **11 September**: Mental Health „Healthy sleep - the right way", de+en
- **10–14 October 2022**: Max Planck Mental Health Awareness Week, de+en
- **18 October**: seminar "The pme range of services for families and individuals"
- **8 November**: pme health day
- **5 October – 2 November**: "Survey on work and management culture and on mental stress"

### 2023

- various Yoga and gymnastics courses
- **7+8 March 2023**: National Day of Healthy Food & Cooking – online
- **17 May**: "Eye relaxation", de+en12 July: "Take a break!", de+en
- **14 September**: Mainz company run
- **10 October**: World Mental Health Day
- **11 October**: Mental Health „Healthy sleep - the right way ", de+en
- **13 December**: "Digital detox - how to succeed in everyday life!", de+en


MPIC Gesundheitswoche / MPIC Health Week 25.05.-28.05.2021
Alkoholkonsum
während der Pandemie
Informationsstand im Erdgeschoss
• Rauschbrillenparcours
Einführung am 26.05.2021, 11:15 Uhr - 15:00 Uhr
• Online-Impulsvortrag – 26.05.2021, 10 Uhr*
„Sober Curious – ein gesundheitsbewusster Lebensstil ohne Alkohol"
• Online-Impulsvortrag – 27.05.2021, 10 Uhr*
„Noch Genuss oder schon Gewohnheit – ein kritischer Blick auf unser Konsumverhalten nicht nur in Coronazeiten"
Den Zoomlink erhalten Sie per Mail.
Alcohol Consumption
during the Pandemic
Information stand on the ground floor
• Intoxication simulation goggles course
Introduction on 26th of May, 11:15 am - 3:00 pm
• Online lecture – 26.05.2021, 10 am*
„Sober Curious – a health-conscious lifestyle without alcohol"
• Online- lecture – 27.05.2021, 10 am*
„Enjoyment or already a habit – a critical look at our consumer behaviour not only in times of corona"
You will receive the zoom link by email.
*The lecture will be held in German.
JOHANNES GUTENBERG UNIVERSITÄT MAINZ
Die Techniker
Diakonie
MPIC Gesundheit
MPIC Health


Tag der gesunden Ernährung
Day of healthy nutrition
Informationsstand im Erdgeschoss.
Information stand on the ground floor.
Online-Vortrag – 08.03.2021, 10-12 Uhr*
„Was ist überhaupt gesunde Ernährung? Eine naturwissenschaftliche Spurensuche"
Von: Prof. Dr. Thomas A. Vilgis, MPI für Polymerforschung, Mainz
Den Zoomlink erhalten Sie per Mail.
*The lecture will be held in German.
MPIC Gesundheit
MPIC Health

## Work safety events

In addition to various online courses the Max Planck Society offers, the institute organized the following events on work safety. During the WORK SAFETY WEEKS, general laboratory and workplace safety training is complemented by specialized sessions such as fire-fighting exercises, rescue training, radiation safety training, as well as cycling safety and the handling of dangerous goods and first aid courses. These courses are customized to the specific needs of laboratories, research campaigns, and the employees.

Once a month: Meeting of the MPIC safety officers

Once a year: laboratory safety checks and check of computer workplaces

### 2021

- **20 July**: Fire safety instructions
- **21 July**: ATTO rescue training
- **16 September**: First Aid Training

### 2022

- **1+5 April**: Safety of handling gas bottles

- **1 June**: Cargo securing in sea containers in accordance with the CTU Code
- **12–16 September**: WORK SAFETY WEEK
- **27 September**: check of computer workplaces and eye examination

### 2023

- **13–17 March**: WORK SAFETY WEEK
- **12 September**: work safety instruction for group leaders
- **11–15 September**: WORK SAFETY WEEK


## Further Gatherings

### Recurring
- Regular German and English classes
- Exchange weeks, organized by the Sustainability Group

### 2021
- **15 April**: Works assembly, online
- **28 September**: Summer party of the works council
- **15 December**: Christmas fundraising event

### 2022
- **21 March**: Fundraising event for Ukraine
- **11+12 June**: Go-Live events for new intranet (in person and online)
- **12 July:** Works assembly
- **15 June**: Summer party
- **14 December**: Christmas fundraising event

### 2023
- **2 February**: New year´s reception
- **21+22 February:** training on construction software (Inventor)
- **23 February**: Fundraising for the victims of the earthquake in Turkey and Syria
- **20 April**: Works assembly
- **18–20 September**: MPG Meeting of engineers and developers
- **30 November**: Christmas reception

# 7 SCIENTIFIC SEMINARS TALKS 2021 – 2023

# 7. SCIENTIFIC SEMINARS TALKS 2021 – 2023

## External Speakers

### 2021

Yuxin Zhou, Lamont-Doherty Earth Observatory, **AMOC instabilities during the last glacial cycle – two case studies** (25 Jan 2021)

Susann Tegtmeier, Institute of Space and Atmospheric Studies, **Atmospheric gas-phase composition over the Indian Ocean** (03 Mar 2021)

Robyn Granger, University Cape Town, **Comparing biogeochemical cycling inside and outside of an Agulhas Ring using nitrogen isotopes in planktic foraminifera** (8 Mar 2021)

Sebastian Flöter, Vrije Universiteit Amsterdam, **The potential of bamboo corals to record environmental conditions in their calcitic skeleton** (12 Apr 2021)

Andreas Kuhn, Biontech, **Development of an mRNA-based vaccine against SARS-CoV-2 at "lightspeed"** (14 Apr 2021)

Benjamin Petrick, Christian Albrechts University Kiel, New **Multi-Million year records of climate change from the shelf of Australia** (26 Apr 2021)

Yael Kiro, Weizmann Institute of Science, **The role of coastal aquifers in ocean chemistry** (10 May 2021)

Lorelei Curtin, University of Wyoming, **Climate and Human History of the Faroe Islands** (31 May 2021)

Ulrich Schumann, DLR, **Strongly reduced air traffic since March 2020 – do we see changes in contrail cirrus and radiative forcing?** (16 Jun 2021)

Christian George, IRCELYON - Institut de Recherches sur la Catalyse et l'Environnement de Lyon, **Photosensitation is in the air and impact its oxidation capacity** (21 Jun 2021)

Peter Hoor, Institute for Atmospheric Physics, JGU, **The Tropopause region in a changing atmosphere** (23 Jun 2021)

Jessica Lueders-Dumont, Smithsonian Tropical Research Institute, Princeton University, **Trophic reconstruction using otolith-bound nitrogen isotopes** (28 Jun 2021)

Sophie Hines, Woods Hole Oceanographic Institution, **Modest changes in Cape Basin glacial ocean structure from benthic carbon and neodymium isotopes** (12 Jul 2021)

Lawrence Percival, Vrije Universiteit Brussel, **From killer trees to stagnant seas: geochemically deciphering the Late Devonian mass extinction** (26 Jul 2021)

Yvan Romé, University of Leeds, **Meltwater driven abrupt climate changes in the North Atlantic simulated in a Heinrich Stadial 1 background** (13 Sep 2021)

Ellen Ai, Princeton/MPIC, **Three modes of change in wind-driven upwelling in the Antarctic Zone during the late-Pleistocene glacial-interglacial cycles** (27 Sep 2021)

Dorothee Moll Thuenen, Institute of Baltic Sea Fisheries, Rostock, **A study on fish habitat connectivity based on otolith microchemistry** (6 Oct 2021)

Niels de Winter, Vrije Universiteit Brussel, **Reconstructing short-term variability during past greenhouse climates** (11 Oct 2021)

Jordan Abell, Arizona State University, **Dust and ATM circulation reconstructions** (25 Oct 2021)

Ralf Eßmann, THW, **Eye witness reports of THW volunteers from the Ahr valley** (3 Nov 2021)

François Fripiat, Université Libre de Bruxelles, Laboratoire de Glaciologie Department Geosciences, **N-isotopes in modern and past oceans** (8 Nov 2021)

Robin Fentimen, University of Fribourg/ ENS Lyon, **East Alboran cold-water coral mounds and their use as palaeoenvironmental archives** (22 Nov 2021)

Philip Pogge von Strandmann, JGU Mainz, **How do you maintain a habitable Earth** (24 Nov 2021)

## 2022

Anne Jantschke, JGU Mainz, **Biomineralization pathways in calcifying dinoflagellates: Uptake, storage in MgCaP-rich bodies and formation of the shell** (19 Jan 2022)

Anja Studer, University of Basel, **First Application of the Diatom-Bound Nitrogen Isotope Paleo-Proxy to Reconstruct Lacustrine Eutrophication** (24 Jan 2022)

Renato Salvatteci, University of Kiel, **A Paleoceanographic perspective on the future of fish productivity in the Humboldt Current System** (7 Feb 2022)

Patrick Blaser, University of Lausanne, **Multi-proxy estimation of glacial and stadial deep Atlantic water mass sourcing** (21 Feb 2022)

Stefan Mulitza, Marum, **Harmonizing foraminiferal proxy data: implications for deglacial changes in global mean sea surface temperature and d18O** (7 Mar 2022)

Mattia Greco, IOPAN, **Decadal trends of the plankton community and habitat shifts in the Arctic gateway recorded by foraminifera** (21 Mar 2022)

Caroline Thaler, LSCE, **Using Geochemistry to reconstruct vital effects** (4 Apr 2022)

David Evans, Frankfurt University, **Earth's climate is not tightly regulated by a silicate weathering feedback** (25 Apr 2022)

Jun-Tae Kim, Korea Inst. Sci. & Technol, R**econstruction of Historical Trends of Long-Range Transport of Anthropogenic Pollutants in the Southern Ocean** (27 Apr 2022)

Alexandra Auderset, MPIC/Princeton, **Enhanced ocean oxygenation during Cenozoic warm periods** (9 May 2022)

Anya Hess, Rutgers University, **Collapse of the East Equatorial Pacific Oxygen Deficient Zone during the Miocene Climatic Optimum** (23 May 2022)

Eva Pfannerstill, University of California, Berkeley, **Airborne eddy covariance flux measurements of Volatile Organic Compounds for constraining air pollution sources and inventories** (24 May 2022)

Martin Hamer, Hochschule Bonn-Rhein-Sieg, **Forschung und Transfer im Rahmen von Citizen Science Projekten – Ein Bsp. aus den Umweltwissenschaften** (1 Jun 2022)

Juan Hofer, Escuela Sciencias del Mar, **Assessing Air-Sea fluxes of climate-relevant trace gases in the Southern Ocean and their effects on atmospheric chemistry** (1 Jun 2022)

Allyiah Akhtar, Princeton University, **Calcium cycling in seawater: insights from isotopic studies of elasmobranch teeth** (13 Jun 2022)

Weiyi Tang, Princeton University, **The impact of wildfires on marine phytoplankton productivity** (27 Jun 2022)

Sarah Shackleton, Princeton University, **Ice cores** (11 Jul 2022)

Matt Sponheimer, University of Colorado Boulder, **The Problem with Paranthropus: deciphering hominin ecology and evolution** (13 Jul 2022)

Katharina Lenhart, TH Bingen, **From a Postdoc position at the MPIC to a professorship at the Bingen Technical University of Applied Sciences – Q&A** (27 Jul 2022)

Samuel Jaccard, University of Lausanne, **The contribution of paleoclimatology to the recent IPCC report** (12 Sep 2022)

Zeynep Erdem, NIOZ, **Paleo-perspectives on the nitrogen cycle in marine upwelling regions** (26 Sep 2022)

Barbara Ervens, University of Clermont Auvergne, **The role of cloud droplet properties in predicting oxidant levels in the atmospheric multiphase system** (28 Sep 2022)

Joshua Fu, University of Tennessee, **Improving Global Estimates of Nitrogen Deposition through Model-Measurement Fusion Approaches** (4 Oct 2022)

Nurit Weber, Weizmann Institute of Science, **Gypsum structures at the shores of the Holocene Dead Sea - Deposition mechanism and paleoclimatic implications** (19 Oct 2022)

Ying Cheng, Paul Scherrer Institute, **Distinguish aerosol's fingerprint on clouds and its relevant climate impact using machine-learning** (9 Nov 2022)

Andreas Herber, **Alfred-Wegener-Institut, Atmospheric airborne campaigns in the Arctic and first operation of the Towed Vehicle T-Bird** (16 Nov 2022)

Mariana Rocha de Souza, University of Hawaii/NOAA, **Coral symbiosis under future ocean conditions** (21 Nov 2022)

Allison Hogikyan, Princeton University, **OMZ modelling** (28 Nov 2022)

Daffne López-Sandoval, King Abdullah University of Science and Technology (KAUST), **Studying phytoplankton metabolic rates at different levels of complexity** (5 Dez 2022)

Yu Wang, ETH Zürich, **How much can atmospheric semivolatile compounds change global clouds?** (7 Dec 2022)

Marietta Straub, **CHUV Lausanne, d15N in cancer tissue** (12 Dec 2022)

## 2023

Julie Meilland, Uni Bremen MARUM, **Asexual reproduction in planktonic foraminifera - the key to evolutionary success and paleoclimate reconstruction** (11 Jan 2023)

Oscar Branson, University of Cambridge, **Boric acid diffusion: implications for biomineralisation and the B geochemical proxies** (16 Jan 2023)

Jassin Petersen, University of Cologne, **The export of barium into the marine benthic realm assessed through Ba/Ca of benthic foraminifera – perspectives from the Aegean Sea** (30 Jan 2023)

Tiziana Durazzano, Università di Genova, **Antarctic Copepod Distributions in the Ross Sea (Antarctica) based on a Machine Learning Modelling Approach** (14 Feb 2023)

Adam Milsom, University of Birmingham, **How does the viscosity, molecular arrangement and composition of surfactant atmospheric aerosol emissions affect the chemical lifetime of aerosol components?** (1 March 2023)

Carsten Sönnichsen, JGU Mainz, **Plasmons as molecular biosensor** (8 Mar 2023)

Michael Tatzel, Georg-August-University Göttingen, **Marine oxygen isotope evolution driven by Chert crystallisation alongside Earth's thermal evolution** (13 Mar 2023)

Neil M. Donahue, Carnegie Mellon University, **How RO2 kinetics got out of the Kugel and into the atmosphere** (20 Mar 2023)

Sonia Chabaane, FRB-Cesab, **Exploring the distribution and diversity of modern planktonic foraminifers under multiple climatic stressors: FORCIS database** (27 Mar 2023)

Gregory Schill, NOAA, **The First Missions with the Next-Generation Particle Analysis by Laser Mass Spectrometry (PALMS-NG) Instrument: Composition of Stratospheric Aerosol in the Asian Tropopause Aerosol Layer and the Northern Hemisphere Polar Vortex** (21 Apr 2023)

Ellen Ai, MPIC/ Princeton University, **Correlation between Southern Ocean front position and wind-driven upwelling during the last deglaciation revealed by (micro)fossil-bound N isotopes** (24 Apr 2023)

Pourya Shahpoury, Trent U & Health Canada, **Oxidative potential - a parameter to assess health risks of ambient particulate matter** (3 May 2023)

Pablo Martínez Sosa, Utrecht University, **GDGTs as a tool to understand dynamic environments** (5 Jun 2023)

Julian Schröder, MPIC/ JGU, **Plio-Arabia: Climate and seasonality of the Arabian deserts during the Pliocene** (5 Aug 2023)

Nicolas Glock, Universität Hamburg, **Adaptations of foraminifera to extreme habitats and related implications for paleo reconstructions of oxygen, nutrients and hydrothermal activity** (7 Sep 2023)

Robert Marks, University of Duisburg Essen, **A powerful new tool for process investigations** (26 Sep 2023)

Jan Jaap Meijer, University of Tasmania, **Meander dynamics in the Antarctic Circumpolar Current** (28 Sep 2023)

Renyi Zhang, College of Arts & Sciences Texas A&M University, **Advancing fundamental atmospheric chemistry by integrating experimental, theoretical, and field studies** (11 Oct 2023)

Marjorie Cantine, University of Washington, **Rapid growth of a carbonate island over the last millennium** (12 Oct 2023)

Ellen Gute, Chalmers University of Technology, **How does it really work – collaboration across and beyond academic disciplines? Learnings from my research and drawing the road ahead for trans-disciplinary research method development** (26 Oct 2023)

Christina Treinen Crespo, University of Baja California, **Marine sediment records reveal the last two centuries of ocean variability in the ETNP** (26 Oct 2023)

Rong Jin, University of Chinese Academy of Sciences, **Halogenated PAHs - an emerging class of pollutants** (8 Nov 2023)

Charlotte Zachow, Universität Tübingen, **How wet is wet? Using strontium isotope ratios to quantify wet intervals in the 115,000-year Chew Bahir Lake record** (09 Nov 2023)

Marloes Penning de Vries, University of Twente, **Invasive weeds in Africa: Everything has its advantages – you just need the right perspective** (15 Nov 2023)

Philipp Franke, FZ Jülich, A**ir quality and emission assessments using 4D-var data assimilation** (12 Dec 2023)

Frauke Logermann, Max Planck Society, **Diversity, Equity & Inclusion: Just a trend or genuine benefit?** (12 Dec 2023)

## Internal Speakers

### 2021

Tina Lüdecke, MPIC, **First enamel nitrogen isotope data of early hominins: Trophic level reconstruction of Australopithecus in the Early Pleistocene (Sterkfontein Member 4, South Africa)** (11 Jan 2021)

Sergey Osipov, MPIC, **Results AQABA Campaign** (27 Jan 2021)

Thomas Berkemeier, MPIC, **Introducing the Chemical Kinetics and Reaction Mechanisms Group** (10 Feb 2023)

Matias Berasategui, MPIC, **Lab kinetics supports interpretation of field observational data** (17 Feb 2021)

Elan Levy, MPIC, **Reconstructing Eastern Mediterranean hydro-climate conditions during the last interglacial from lake and speleothem records** (22 Feb 2021)

Ivan Tadic, MPIC, **Central role of NO in ozone production in the upper tropical troposphere over the Atlantic Ocean and West Africa** (17 Mar 2021)

Anna Kunert, MPIC, **Atmospheric ice nucleation: basics, instrument development and application** (31 Mar 2021)

Benjamin Bandowe, MPIC, **On the sources, fate and adverse effects of polycyclic aromatic compounds** (21 Apr 2021)

Daniel Marno, MPIC, **The Oxidation Capacity of the Summertime Asian Monsoon Anticyclone** (28 Apr 2021)

Jan Leitner, MPIC, **NanoSIMS applications in Climate Geochemistry: High-resolution trace element studies of foraminiferal shells** (5 May 2021)

Kurt Lucas, MPIC, **Molecular Aspects of Inflammation - including new suggestion for the treatment of COVID-19 and Post-COVID** (12 May 2021)

Tina Luedecke, MPIC, **The Onset and Evolution of Early Hominin Meat Consumption (HoMeCo)** (19 May 2021)

Jan David Förster, MPIC, **X-ray microspectroscopy in the analysis of atmospheric and respiratory aerosols** (26 May 2021)

Kathryn Fitzsimmons, MPIC, **Quantifying long-term climate change in Central Asia - the Research Group for Terrestrial Palaeoclimates, nearly 5 years on** (2 Jun 2021)

Zaneta Hamryszczak, MPIC, **Distribution of Hydroperoxides over Europe during CAFE-EU/BLUESKY campaign** (9 Jun 2021)

Christian Borger, MPIC, **Analysis of global trends of total column water vapour from multiple years of OMI observations** (7 Jul 2021)

Eleni Dovrou, MPIC, **The contribution of H2O2 and reactive organic carbon to formation of particulate matter and to oxidative stress in the respiratory tract** (preliminary) (21 Jul 2021)

Friederike Fachinger, MPIC, **How villages contribute to their local air quality – the influence of traffic- and biomass combustion-related emissions assessed by mobile mappings of PM and its components** (18 Aug 2021)

Clara Nussbaumer, MPIC, **Photochemical production and loss rates of formaldehyde and ozone across Europe** (25 Aug 2021)

Kathrin Reinmuth-Selzle, MPIC, **Protein analysis of complex samples and chemically modified allergens: analytical challenges & health effects** (8 Sept 2021)

Roland Rohloff, MPIC, **Impact of convective outflow on the oxidation capacity in the upper troposphere studied during Café Africa** (22 Sept 2021)

Marco Wietzoreck, MPIC, **Polycyclic aromatic compounds - oxidative potential and inhalation bioaccessibility** (13 Oct 2021)

Kurt Lucas, MPIC, **Therapeutic Use of Hydrogen (H2)** (20 Oct 2021)

Olli Eppers, MPIC, **Chemical composition of cloud-interacting aerosol particles in the Arctic summer** (8 Dec 2021)

## 2022

Sven Brömme, JGU/MPIC, **Tracing the Laacher See climatic imprint in late glacial Swiss pine trees** (10 Jan 2022)

Vinod Kumar, MPIC, **Overview of high-resolution atmospheric chemistry modelling activities for supporting satellite and ground-based measurements** (12 Jan 2022)

Kurt Lucas, MPIC, **Sex- und Familienleben der Pflanzen, Untertitel „Generationswechsel und Organisation des Pflanzenreichs in Familien** (26 Jan 2022)

Frank Helleis, MPIC, **Update Ventilation Strategies** (2 Feb 2022)

Patrick Dewald, MPIC, **NO3 reactivity during TO2021 at the Kleiner Feldberg** (16 Feb 2022)

Janos Kodolanyi, MPIC, **The short-lived radioactive isotope 60Fe in the early Solar System: a NanoSIMS-TEM investigation of ancient meteorites** (23 Feb 2022)

Marco Linke/ Norman Eschenfelder, MPIC, **1 Jahr Matrix42 am MPIC** (2 Mar 2022)

Lenard Röder, MPIC, **Sequential Monte Carlo Filters for Atmospheric Chemistry Field Experiments** (9 Mar 2022)

Florian Reyzek, MPIC, **Purification and characterization of ice nuclei from birch pollen** (16 Mar 2022)

Guangjie Zheng, MPIC, **New particle formation in the remote marine boundary layer** (30 Mar 2022)

Kurt Lucas, MPIC, **Molecular Feedback Loops During Inflammation** (20 Apr 2022)

Alan Foreman, MPIC, **Overview of sampling activities in the Equatorial Pacific in 2020/2021 to reconstruct the variability of the Oxygen Minimum Zones over the past century** (11 May 2022)

Jennifer Schallock, MPIC, **Model Simulations of Stratospheric Aerosol: Volcanic Eruptions, Sulfur Chemistry and Evaluation with Field Data Campaign** (18 May 2022)

Monika Markowska, MPIC, **Saudi Arabian stalagmites: How do they record the drying of the Arabian peninsula over the past 3 mio years** (25 May 2022)

Moritz Schöne, MPIC, **Satellite observations of tropospheric BrO plumes in polar spring and comparison to WRF-Chem model results** (8 Jun 2022)

Jennifer Leichliter, MPIC, **A new proxy for reconstructing ancient food webs: Nitrogen isotopes in tooth enamel** (29 Jun 2022)

Meng Li, MPIC, **Photochemical aging of soot by $O_2$** (20 Jul 2022)

Julia Pikmann, MPIC, **Influence of preparation method, activities during cooking and ingredients on chemical and physical properties of the emitted aerosol** (10 Aug 2022)

Dirk Dienhart, MPIC, **Formaldehyde and hydroperoxide measurements during AQABA** (17 Aug 2022)

Gerhard Lammel, MPIC, **Global chemical pollution an ongoing trend of global environmental change** (24 Aug 2022)

Maayan Yehudai, MPIC, **Controls of North Atlantic nitrogen fixation over the Pliocene-Pleistocene transition** (12 Oct 2022)

Paul Zander, MPIC, **Hyperspectral imaging sediment core scanning for biogeochemical analysis** (31 Oct 2022)

Anna Shapiro, Max Planck Institute for Solar System Research, **Planetary UV radiation stress to life intensifies with stellar metallicity** (26 Oct 2022)

Hubert Vonhof, MPIC, **Stalagmites as a continental paleoclimate archive** (2 Nov 2022)

Janine Fröhlich, MPIC, **Chemical modification and TLR4 activation of the grass pollen allergen Phl p 5.** (23 Nov 2022)

Steven Lelieveld, MPIC, **Reactive oxygen species in the lung: Kinetic modeling of air pollution induced oxidative stress** (30 Nov 2022)

## 2023

Linda Ort, MPIC, **Forschung und Leben auf dem Eis – Mein Jahr in der Antarktis** (22 Feb 2023)

Martin Carswell, MPIC, **Export Control & Shipping Presentation** (4 Mar 2023)

Kurt Lucas, MPIC, **Molecular Aspects of Inflammation and Allergies – Insights into the Work of AG Lucas** (5 Apr 2023)

Jan Leitner, MPIC, **New Isotopic Insights into the Solar System's Circumstellar Building Blocks** (12 Apr 2023)

Sergey Gromov, MPIC, **Past atmospheric chemistry variations: model-aided novel-proxy investigation since the Last Glacial Maximum** (17 May 2023)

Oliver Eppers, MPIC, **Chemical composition and processing of aerosol particles in the Asian Tropopause Aerosol Layer inferred from airborne measurements during the ACCLIP campaign** (07 Jun 2023)

Maayan Yehudai, MPIC, **A mental-health crisis is gripping science** (19 Jun 2023)

Simon Warnach, MPIC, **A global perspective on the BrO/SO2 ratio inside volcanic gas plumes – insights into volcanic and atmospheric processes** (21 Jun 2023)

Sven Brömme, MPIC, **Inter- and intra-tooth variability in enamel-bound nitrogen isotopic composition. A case study from Gorongosa National Park, Mozambique** (6 Jul 2023)

Kurt Lucas, MPIC, **Long Covid: state of research** (02 Aug 2023)

Clara Nussbaumer, MPIC, **$O_3$ sensitivity towards $NO_x$ and VOCs throughout the troposphere – a new indicator $\alpha(CH_3O_2)$** (09 Aug 2023)

Elan Levy, MPIC/Geological Survey of Israel, **Chemical composition and processing of aerosol particles in the Asian Tropopause Aerosol Layer inferred from airborne measurements during the ACCLIP campaign** (30 Aug 2023)

Marissa Vink, MPIC, **Intra-tooth variation of stable carbon, nitrogen, and oxygen isotopes in fossil tooth enamel of equids from the Middle Paleolithic site of Neumark-Nord 2, Germany** (14 Sep 2023)

Matthias Kohl, MPIC, **(Ultrafine) particles in the atmosphere - a modelling perspective** (27 Sept 2023)

Alan Foreman, MPIC, **Expansion of the Indian Ocean Subtropical Gyre across the 20th Century** (4 Oct 2023)

# 8 SCIENTIFIC PUBLICATIONS 2021–2023

## INCLUDING DOCTORAL, MASTER AND BACHELOR THESES

# 8. SCIENTIFIC PUBLICATIONS 2021–2023

**The initial section of the publications lists Doctoral, Master, and Bachelor theses according to departments and independent research groups, followed by the second part, encompassing all Journal Articles, Books, and Book chapters published in the years 2021–2023.**

## DOCTORAL THESES

### ATMOSPHERIC CHEMISTRY DEPARTMENT – J. Lelieveld

#### Year 2023

Dienhart, D.: Atmospheric oxidation precursors in the marine boundary layer around the Arabian Peninsula, Doctoral thesis, Mainz University, 2023.

Dörich, R.: Luft- und bodengestützte Spurengasmessungen von Peroxyacetylnitraten (PANs) und Peressigsäure (PAA) mittels Massenspektrometrie über chemische Ionisation mit Iodid Ionen, Doctoral thesis, Mainz University, 2023.

Hamryszczak, Z. T.: Hydroperoxide measurements in outdoor environments, Doctoral thesis, Mainz University, 2023.

Nussbaumer, C. M.: Nitrogen oxides and their involvement in photochemical processes throughout the troposphere, Doctoral thesis, Mainz University, 2023.

Tauer, S. M.: The oxidative capacity of the atmosphere around the Arabian Peninsula: Ship-based atmospheric measurements of OH and HO2 radicals using laser induced fluorescence spectroscopy, Doctoral thesis, Mainz University, 2023.

#### Year 2022

Byron, J.: Investigating Biogenic Sources of Enantiomers and the Effect of Drought on the Emissions of Chiral Compounds. Doctoral thesis, Mainz University, 2022.

Dewald, P.: Chamber and field studies on NO3 reactivity and the detection of alkyl nitrates during the NO3-induced oxidation of isoprene and terpenes, Doctoral thesis, Mainz University, 2022.

Rohloff, R.: Konvektiver Einfluss auf das OH-Oxidationspotential der oberen tropischen Troposphäre, Doctoral thesis, Mainz University, 2022.

#### Year 2021

Friedrich, N.: The reactive nitrogen budget throughout the diel cycle investigated via thermal dissociation cavity ring-down spectroscopy, Doctoral thesis, Mainz University, 2021.

Li, M.: Trends of atmospheric radicals, trace gases and their residence time, Doctoral thesis, Mainz University, 2021.

Marno, D. R.: The Oxidation Capacity of the Summertime Asian Monsoon Anticyclone - Airborne measurements of OH and HO2 radicals in the Upper Troposphere using Laser Induced Fluorescence Spectroscopy, Doctoral thesis, Mainz University, 2021.

Schallock, J.: Stratospheric Aerosol: Budgets, Chemistry and radiative Transfer based on a complex Chemistry Climate Model and Satellite and Field Campaign Data, Doctoral thesis, Mainz University, 2021.

Wang, N.: Carbonyl compounds and their OH reactivities in outdoor and indoor environments, Doctoral thesis, Mainz University, 2021.

### CLIMATE GEOCHEMISTRY DEPARTMENT – G. H. Haug

#### Year 2023

Wald, T.: The Nitrogen Cycle in the Mediterranean Sea, Doctoral thesis, ETH, Zürich, 2023.

#### Year 2021

Moretti, S.: Application of fossil-bound nitrogen isotopes to the reconstruction of the marine nitrogen cycle dynamics during warming and cooling phases in Earth's Cenozoic history, Doctoral thesis, ETH, Zürich. 2021.

## MULTIPHASE CHEMISTRY DEPARTMENT – U. Pöschl

### Year 2023

Lauer, O.: Aerosol effects on microphysical properties of Amazonian clouds, Doctoral thesis, Mainz University, 2023.

Rösch, M.: A novel effervescent hydrogen-generating tablet – formulation, optimization and in-depth characterization, Doctoral thesis, Mainz University, 2023.

### Year 2022

Lelieveld, S.: Reactive oxygen species in epithelial lining fluid: Kinetic modeling of air pollution induced oxidative stress, Doctoral thesis, Mainz University, 2022.

Prass, M.: Bioaerosols in the Amazon characterized by molecular- genetic staining techniques, Doctoral thesis, Mainz University, 2022.

Wietzoreck, M.: Nitro- and oxyaromatic compounds: environmental cycling and exposure, Doctoral thesis, Mainz University, 2022.

### Year 2021

Filippi, A.: EPR Measurements and Redox Chemistry of Fine Particulate Matter, Doctoral thesis, Mainz University, 2021.

Holanda, B. A.: Atmospheric processing and relevance of biomass burning aerosols over the Amazon and the Atlantic, Doctoral thesis, Mainz University, 2021.

Kratz, A.: Relevance of biological soil crusts in biogeochemical cycling, Doctoral thesis, Mainz University, 2021.

Kunert, A. T.: Protein interactions related to biological ice nucleation allergies and inflammation, Doctoral thesis, Mainz University, 2021.

Wilson, J.: Multiphase chemistry and partitioning of PAHs: numerical modeling from molecular to global scales, Doctoral thesis, Mainz University, 2021.

## PARTICLE CHEMISTRY DEPARTMENT – S. Borrmann

### Year 2023

Kaiser, K.: Chemical composition and transformation of submicron aerosol particles in the outflow of large major population centers, Doctoral thesis, Mainz University, 2023.

Pikmann, J.:, Untersuchung gesundheitsrelevanter Aerosole mit Schwerpunkt auf Kochaktivitäten, Doctoral thesis, Mainz University, 2023.

### Year 2022

Clemen, H.-C.: Weiterentwicklung eines Einzelpartikel-Massenspektrometers und dessen Anwendung auf Aerosolpartikel, Eiskeime und Eispartikelresiduen in der freien Troposphäre, Doctoral thesis, Mainz University, 2022.

### Year 2021

Eppers, O.: Chemical composition and origin of aerosol particles involved in summertime Arctic cloud processes, Doctoral thesis, Mainz University, 2021.

Port, M.: Flugzeuggetragene Messungen von Eis- und Zirruswolken im Troposphären-Stratosphären Übergangsbereich des Asiatischen Sommermonsuns, Doctoral thesis, Mainz University, 2021.

## INDEPENDENT RESEARCH GROUPS

### Aerosols & Regional Air Quality Group – Y. Cheng

#### Year 2022

Chen, C.: Nano-size Effect on Phase Transition of Atmospheric Aerosol Particles, Doctoral thesis, Mainz University, 2022.

#### Year 2021

Lei, T.: Size dependent hygroscopicity of aerosol nanoparticles, Doctoral thesis, Mainz University, 2021.

Liu, L.: Impact of aerosols on cloud and precipitation in the Amazon, Doctoral thesis, Mainz University, 2021.

### Satellite Remote Sensing Group – T. Wagner

#### Year 2023

Schöne, M: Tropospheric BrO plumes in Arctic spring – A comparison of TROPOMI satellite observations and model results, Doctoral thesis, Heidelberg, doi:10.11588/heidok.00032838, 2023.

#### Year 2022

Borger, C.: Long-term analysis of the global water vapour distribution based on satellite measurements; Doctoral thesis, Mainz, doi:10.25358/openscience-9062, 2022.

Razi, M.: Measurement of Nitrogen Dioxide, Sulphur Dioxide, Formaldehyde and Glyoxal by Using Car MAX-DOAS Observations in and around the Megacity of Lahore, Pakistan, Doctoral thesis, doi:10.25358/openscience-6796, 2022.

Warnach, S.: Bromine monoxide in volcanic plumes - A global survey of volcanic plume composition and chemistry derived from Sentinel-5 Precursor/TROPOMI data, Doctoral thesis, Heidelberg, doi:10.11588/heidok.00031910, 2022.

### Terrestrial Palaeoclimates – K. Fitzsimmons (group until 2021)

#### Year 2022

Dave, A. K.: Understanding Quaternary aeolian landscape-climate interaction in the piedmonts of Central Asia using luminescence and electron spin resonance techniques, Doctoral thesis, Mainz University, 2022.

# MASTER THESES

## ATMOSPHERIC CHEMISTRY DEPARTMENT – J. Lelieveld

### Year 2023

Fernholz, C.: Untersuchung der Kinetik der Reaktion zwischen Methylnitrat und dem Hydroxylradical mittels Laserphotolyse / Laserinduzierter Fluoreszenz, Master thesis, Würzburg, 2023.

Türk, G. N. T. E.: Softwareentwicklung und die erste Messung eines Cavity Ring-Down Spektrometers für NO3, Master thesis, Mainz, 2023.

Wüst, L.: Charakterisierung des Einflusses von Stockoxiden und Ozon auf die Quantifizierung biogener organischer Nitrate mittels Thermischer-Dissoziations Cavity-Ring-Down Spektroskopie, Master thesis, Mainz, 2023.

## PARTICLE CHEMISTRY DEPARTMENT – S. Borrmann

### Year 2023

Büttner, M.: Characterization of the laboratory version of the Ultra-High Sensitivity Aerosol Spectrometer with respect to aircraft operation, Master thesis, University Mainz, 2023.

Junk, N.: Charakterisierung des Potential Aerosol Mass (PAM) Oxidation Flowreactor, Master thesis, University Mainz, 2023.

### Year 2022

Champion, N.: Olivine with sulfuric acid coating as an analogue of stratospheric meteoric aerosol for the ERICA Laser Ablation Mass Spectrometer, Master thesis, University Mainz, 2022.

Grzegorczyk, P.: Exploring the role of fragmentation of ice particles by laboratory studies, MASTER STPE, parcours Sciences de l'Atmosphère et du Climat Ecole OPGC, Master thesis, Université Clermont Auvergne, betreut am Mainzer Vertikalwindkanal, 2022.

Mouji. N.: Analysis of biomass burning plumes encountered during the NETCARE flight measurement campaign in 2014: Particle composition, sources, and transport pathways into the Arctic, Master thesis, University Mainz, 2022.

## INDEPENDENT RESEARCH GROUPS

## Satellite Remote Sensing Group – T. Wagner

### Year 2023

Bastani, E.: Detection of clouds by infrared measurements from the ground. Master thesis, Mainz, 2023.

### Year 2022

Rall, A. A.: Effekt von Wolken auf die schräge Säulendichte vom Sauerstoff-Dimer, gemessen mit zenithen DOAS Himmelsmessungen, Master thesis, Heidelberg., 2022.

### Year 2021

Lukosiunaite, S.: Deriving Nitrogen Oxide emissions from inland waterway vessels using MAX-DOAS measurements, Master thesis, Mainz, 2021.

# BACHELOR THESES

## ATMOSPHERIC CHEMISTRY DEPARTMENT – J. Lelieveld

### Year 2022

Hartmann, A.: Optimierung der Konversionseffizienz eines photolytischen Konverters zur Stickoxidmessung. Bachelor thesis, Mainz, 2022.

## PARTICLE CHEMISTRY DEPARTMENT – S. Borrmann

### Year 2022

Arndt, A.: Eine Windkanalstudie zur Bestimmung des Retentionskoeffizienten von Pinonsäure an bereifenden Graupeln unter trockenen Wachstumsbedingungen, Bachelor thesis, Mainz, 2022.

Gömmer, L.: Eine Windkanalstudie zur Bestimmung des Retentionskoeffizienten von Pinonsäure während der Bereifung im Nasswachstum, Bachelor thesis, Mainz, 2022.

Hey, M.: Experimentelles Bestimmen der Verteilungskoeffizienten wässriger Malonsäure-lösungen, Bachelor thesis, Mainz, 2022

### Year 2021

Zanger, F.: Herstellung, Charakterisierung und aerodynamische Eigenschaften von Graupel, Bachelor thesis, Mainz, 2021.

## INDEPENDENT RESEARCH GROUPS

### Satellite Remote Sensing Group – T. Wagner

### Year 2022

Rentel, D. S.: The relationship of volcanic emissions to the seismic activity of the Etna volcano, Bachelor thesis, Mainz. 2022.

Volkers, J.: Examination of the O4-scaling factor for MAX-DOAS profile inversions, Bachelor thesis, Heidelberg. 2022.

### Year 2021

Jost, A: The relationship of volcanic emissions to the seismic activity of the Etna volcano. Bachelor thesis, Mainz, 2021.

# SCIENTIFIC PAPER

## ATMOSPHERIC CHEMISTRY DEPARTMENT – J. Lelieveld

## JOURNAL ARTICLES

### Year 2023


Abdelkader, M., Stenchikov, G., Pozzer, A., Tost, H. and Lelieveld, J.: The effect of ash, water vapor, and heterogeneous chemistry on the evolution of a Pinatubo-size volcanic cloud, Atmospheric Chemistry and Physics, 23(1), 471–500, doi:10.5194/acp-23-471-2023, 2023.

Alves, E. G., Santana, R. A., Dias-Júnior, C. Q., Botía, S., Taylor, T., Yáñez-Serrano, A. M., Kesselmeier, J., Bourtsoukidis, E., Williams, J., de Assis, P. I. L. S., Martins, G., de Souza, R., Júnior, S. D., Guenther, A., Gu, D., Tsokankunku, A., Sörgel, M., Nelson, B., Pinto, D., Komiya, S., Rosa, D. M., Weber, B., Barbosa, C., Robin, M., Feeley, K. J., Duque, A., Lemos, V. L., Contreras, M. P., Idarraga, A., López, N., Husby, C., Jestrow, B. and Toro, I. M. C.: Intra- and interannual changes in isoprene emission from central Amazonia, Atmospheric Chemistry and Physics, 23(14), 8149–8168, doi:10.5194/acp-23-8149-2023, 2023.

Bensemann, J., Cheena, H., Huang, D. T. J., Broadbent, E., Williams, J. and Wicker, J.: From What You See to What We Smell: Linking Human Emotions to Bio-markers in Breath, IEEE transactions on affective computing, doi:10.1109/TAFFC.2023.3275216., 2023.

Carlsson, P. T. M., Vereecken, L., Novelli, A., Bernard, F., Brown, S. S., Brownwood, B., Cho, C., Crowley, J. N., Dewald, P., Edwards, P. M., Friedrich, N., Fry, J. L., Hallquist, M., Hantschke, L., Hohaus, T., Kang, S., Liebmann, J., Mayhew, A. W., Mentel, T., Reimer, D., Rohrer, F., Shenolikar, J., Tillmann, R., Tsiligiannis, E., Wu, R., Wahner, A., Kiendler-Scharr, A. and Fuchs, H.: Comparison of isoprene chemical mechanisms under atmospheric night-time conditions in chamber experiments: evidence of hydroperoxy aldehydes and epoxy products from NO3 oxidation, Atmospheric Chemistry and Physics, 23(5), 3147–3180, doi:10.5194/acp-23-3147-2023, 2023.

Chowdhury, S., Pillarisetti, A., Oberholzer, A., Jetter, J., Mitchell, J., Cappuccilli, E., Aamaas, B., Aunan, K., Pozzer, A. and Alexander, D.: A global review of the state of the evidence of household air pollution's contribution to ambient fine particulate matter and their related health impacts, Environment International, 173, doi:10.1016/j.envint.2023.107835, 2023.

Christou, M., Koyutourk, B., Yetismis, K., Martinou, A. F., Christodoulou, V., Koliou, M., Antoniou, M., Pavlou, C., Ozbel, Y., Kasap, O. E., Alten, B., Georgiades, P., Georgiou, G. K., Christoudias, T., Proestos, Y., Lelieveld, J. and Erguler, K.: Entomological surveillance and spatiotemporal risk assessment of sand fly-borne diseases in Cyprus, Current research in parasitology & vector-borne diseases, 4, doi:10.1016/j.crpvbd.2023.100152, 2023.

Dewald, P., Lelieveld, J. and Crowley, J. N.: NO3 reactivity measurements in an indoor environment: a pilot study, Environmental science: Atmospheres, doi:10.1039/D3EA00137G, 2023.

Dienhart, D., Brendel, B., Crowley, J. N., Eger, P. G., Harder, H., Martinez, M., Pozzer, A., Rohloff, R., Schuladen, J., Tauer, S., Walter, D., Lelieveld, J. and Fischer, H.: Formaldehyde and hydroperoxide distribution around the Arabian Peninsula – evaluation of EMAC model results with ship-based measurements, Atmospheric Chemistry and Physics, 23(1), 119–142, doi:10.5194/acp-23-119-2023, 2023.

Dovrou, E., Lelieveld, S., Mishra, A., Pöschl, U. and Berkemeier, T.: Influence of ambient and endogenous H2O2 on reactive oxygen species concentrations and OH radical production in the respiratory tract, Environmental science: Atmospheres, doi:10.1039/D2EA00179A, 2023.

Economou, T., Lazoglou, G., Tzyrkalli, A., Constantinidou, K. and Lelieveld, J.: A data integration framework for spatial interpolation of temperature observations using climate model data, PeerJ Life & Environment, 11, doi:10.7717/peerj.14519, 2023.

Ernle, L., Ringsdorf, M. A. and Williams, J.: Influence of ozone and humidity on PTR-MS and GC-MS VOC measurements with and without a Na2S2O3 ozone scrubber, Atmospheric Measurement Techniques, 16(5), 1179–1194, doi:10.5194/amt-16-1179-2023, 2023.

Ernle, L., Wang, N., Bekoe, G., Morrison, G., Wargocki, P., Weschler, C. J. J. and Williams, J.: Assessment of aldehyde contributions to PTR-MS m/z 69.07 in indoor air measurements, Environmental science: Atmospheres, doi:10.1039/d3ea00055a, 2023.

Georgiades, P., Proestos, Y., Lelieveld, J. and Erguler, K.: Machine Learning Modeling of Aedes albopictus Habitat Suitability in the 21st Century, Insects, 14(5), doi:10.3390/insects14050447, 2023.

Gurriaran, L., Tanaka, K., Bayram, S., Proestos, Y., Lelieveld, J. and Ciais, P.: Warming-induced increase in power demand and CO2 emissions in Qatar and the Middle East, Journal of Cleaner Production, 382, doi:10.1016/j.jclepro.2022.135359, 2023.

Hadjinicolaou, P., Tzyrkalli, A., Zittis, G. and Lelieveld, J.: Urbanisation and Geographical Signatures in Observed Air Temperature Station Trends Over the Mediterranean and the Middle East–North Africa, Earth systems and environment, 7, doi:10.1007/s41748-023-00348-y, 2023.

Hahad, O., Rajagopalan, S., Lelieveld, J., Sørensen, M., Frenis, K., Daiber, A., Basner, M., Nieuwenhuijsen, M., Brook, R. D. and Münzel, T.: Noise and Air Pollution as Risk Factors for Hypertension: Part I—Epidemiology, Hypertension, 80, 983–988, doi:10.1161/HYPERTENSIONAHA.122.18732, 2023.

Hahad, O., Rajagopalan, S., Lelieveld, J., Sørensen, M., Kuntic, M., Daiber, A., Basner, M., Nieuwenhuijsen, M., Brook, R. D. and Münzel, T.: Noise and Air Pollution as Risk Factors for Hypertension: Part II—Pathophysiologic Insight, Hypertension, 80, 1384–1392, doi:10.1161/HYPERTENSIONAHA.123.20617, 2023.

Hajat, S., Proestos, Y., Araya-Lopez, J.-L., Economou, T. and Lelieveld, J.: Current and future trends in heat-related mortality in the MENA region: a health impact assessment with bias-adjusted statistically downscaled CMIP6 (SSP-based) data and Bayesian inference, Lancet Planetary Health, 7(4), E282–E290, doi:10.1016/S2542-5196(23)00045-1, 2023.

Hamryszczak, Z., Dienhart, D., Brendel, B., Rohloff, R., Marno, D., Martinez, M., Harder, H., Pozzer, A., Bohn, B., Zöger, M., Lelieveld, J. and Fischer, H.: Measurement report: Hydrogen peroxide in the upper tropical troposphere over the Atlantic Ocean and western Africa during the CAFE-Africa aircraft campaign, Atmospheric Chemistry and Physics, 23(10), 5929–5943, doi:10.5194/acp-23-5929-2023, 2023.

von Hobe, M., Brühl, C., Lennartz, S. T., Whelan, M. E. and Kaushik, A.: Comment on "An approach to sulfate geoengineering with surface emissions of carbonyl sulfide" by Quaglia et al. (2022), Atmospheric Chemistry and Physics, 23(11), 6591–6598, doi:10.5194/acp-23-6591-2023, 2023.

Holanda, B. A., Franco, M. A., Walter, D., Artaxo, P., Carbone, S., Cheng, Y., Chowdhury, S., Ditas, F., Gysel-Beer, M., Klimach, T., Kremper, L. A., Krüger, O. O., Lavric, J. V., Lelieveld, J., Ma, C., Machado, L. A. T., Modini, R. L., Morais, F. G., Pozzer, A., Saturno, J., Su, H., Wendisch, M., Wolff, S., Pöhlker, M. L., Andreae, M. O., Pöschl, U. and Pöhlker, C.: African biomass burning affects aerosol cycling over the Amazon, Communications Earth & Environment, 4, doi:10.1038/s43247-023-00795-5, 2023.

Jiang, Y., Hoffmann, E. H., Tilgner, A., Aiyuk, M. B. E., Andersen, S. T., Wen, L., van Pinxteren, M., Shen, H., Xue, L., Wang, W. and Herrmann, H.: Insights Into NOxand HONO Chemistry in the Tropical Marine Boundary Layer at Cape Verde During the MarParCloud Campaign, Journal of Geophysical Research: Atmospheres, 128(16), doi:10.1029/2023JD038865, 2023.

Karu, E., Li, M., Ernle, L., Brenninkmeijer, C. A. M., Lelieveld, J. and Williams, J.: Carbonyl Sulfide (OCS) in the Upper Troposphere/Lowermost Stratosphere (UT/LMS) Region: Estimates of Lifetimes and Fluxes, Geophysical Research Letters, 50(19), doi:10.1029/2023GL105826, 2023.

Kaskaoutis, D. G., Pikridas, M., Barmpounis, K., Kassell, G., Logan, D., Rigler, M., Ivancic, M., Mohammadpour, K., Mihalopoulos, N., Lelieveld, J. and Sciare, J.: Aerosol characteristics and types in the marine environments surrounding the East Mediterranean- Middle East (EMME) region during the AQABA campaign, Atmospheric Environment, 298, doi:10.1016/j.atmosenv.2023.119633, 2023.

Keller, K., Haghi, S. H. R., Hahad, O., Schmidtmann, I., Chowdhury, S., Lelieveld, J., Münzel, T. and Hobohm, L.: Air pollution impacts on in-hospital case-fatality rate of ischemic stroke patients, Thrombosis Research, 225, 116–125, doi:10.1016/j.thromres.2023.03.006, 2023.

Khomenko, S., Pisoni, E., Thunis, P., Bessagnet, B., Cirach, M., Iungman, T., Barboza, E. P., Khreis, H., Mueller, N., Tonne, C., de Hoogh, K., Hoek, G., Chowdhury, S., Lelieveld, J. and Nieuwenhuijsen, M.: Spatial and sector-specific contributions of emissions to ambient air pollution and mortality in European cities: a health impact assessment, Lancet Public Health, 8(7), e546–e558, doi:10.1016/S2468-2667(23)00106-8, 2023.

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## CLIMATE GEOCHEMISTRY DEPARTMENT – G. H. Haug

## JOURNAL ARTICLES

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# SCIENTIFIC PAPER

## MULTIPHASE CHEMISTRY DEPARTMENT – U. Pöschl

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# SCIENTIFIC PAPER

## INDEPENDENT RESEARCH GROUPS

### Aerosols & Regional Air Quality Group – Y. Cheng

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# High Pressure Chemistry and Physics Group – M. Eremets

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## Hominin Meat Consumption – T. Lüdecke

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## Satellite Remote Sensing Group – T. Wagner

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## Terrestrial Palaeoclimates – K. Fitzsimmons (group until 2021)

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# 9 PUBLICATIONS ANALYSES

# Publication Output and Citation Impact

**A bibliometric analysis of the MPI for Chemistry, Mainz, in the publication period 2012-2022**

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**Introduction:** The bibliometric analysis of the MPI for Chemistry in Mainz (MPIC) deals with the research performance of the institute during the publication period 2012-2022. The methods used and the presentation and interpretation of the results follow the "Standards for the application of bibliometrics in the evaluation of research institutes in the field of natural sciences" (Bornmann et al., 2012; Bornmann et al., 2014; Hicks, Wouters, Waltman, de Rijcke, and Rafols, 2015) and considers the recommendations for research evaluation studies of Marx (2011), Marx and Bornmann (2012), Bornmann and Haunschild (2017), and Haunschild, Schier, and Bornmann (2016).

**Data set:** The mission of the Max Planck Institutes is to conduct basic research. The result of the research activities is therefore mainly publications in scientific journals. The number of publications (henceforth also referred to as "papers" or "publications" interchangeably rather than articles, in order to avoid confusion with the document type "article") that have appeared in peer-reviewed journals covered by Clarivate Analytics' Web of Science (WoS) has become the standard reference for the quantification of scientific output (Birkle, Pendlebury, Schnell, and Adams, 2020). The MPIC publications were identified by the authors' addresses: All publications were selected in which this Max Planck Institute was stated as an author's address. This publication set has been checked by the local library. They indicated 103 papers to be removed in which the MPIC address has not been the primary affiliation of the respective MPIC author or whose authors have no longer been employed by the MPIC. Eleven additional papers have been included that lack an indexed MPIC address in the WoS but were indicated by the institute as affiliated with the MPIC. The data used in this analysis stem – if not otherwise noted – from a bibliometrics database developed and maintained in cooperation with the Max Planck Digital Library (MPDL, Munich) and derived from the Science Citation Index – Expanded (SCI-E), the Social Sciences Citation Index (SSCI), the Conference Proceedings Citation Index – Science (CPCI-S), the Conference Proceedings Citation Index – Social Science & Humanities (CPCI-

SSH), and the Arts and Humanities Citation Index (AHCI), provided by Clarivate Analytics and updated in calendar week 24 in 2023.

This study deals with publications of the MPIC from 2012 to 2022 of the document types “article” and “review” (and the corresponding citation metrics). It is a standard procedure in bibliometrics to exclude publications of other document types from the statistical analyses. For each publication, the citation impact has been measured from the publication year until the end of 2022.

**Publication output:** Out of the total of 2,406 publications published by the MPI, 2,317 (96.3%) belong to the document type “article”, and 89 (3.7%) to “review”. According to the WoS web-interface, 75.9% (n=1,826) of the total set are Open Access papers. Figure 1 shows the distribution of the publications across the publication years 2012 to 2022. According to the figure, the MPI publishes on average about 219 publications per year (black line in Figure 1). On average, the output has been slightly increasing over the years. About 88.0% (n=2,118) of the papers have been written as international cooperations. Appendix A includes more information about collaborations of the MPIC on a country basis.

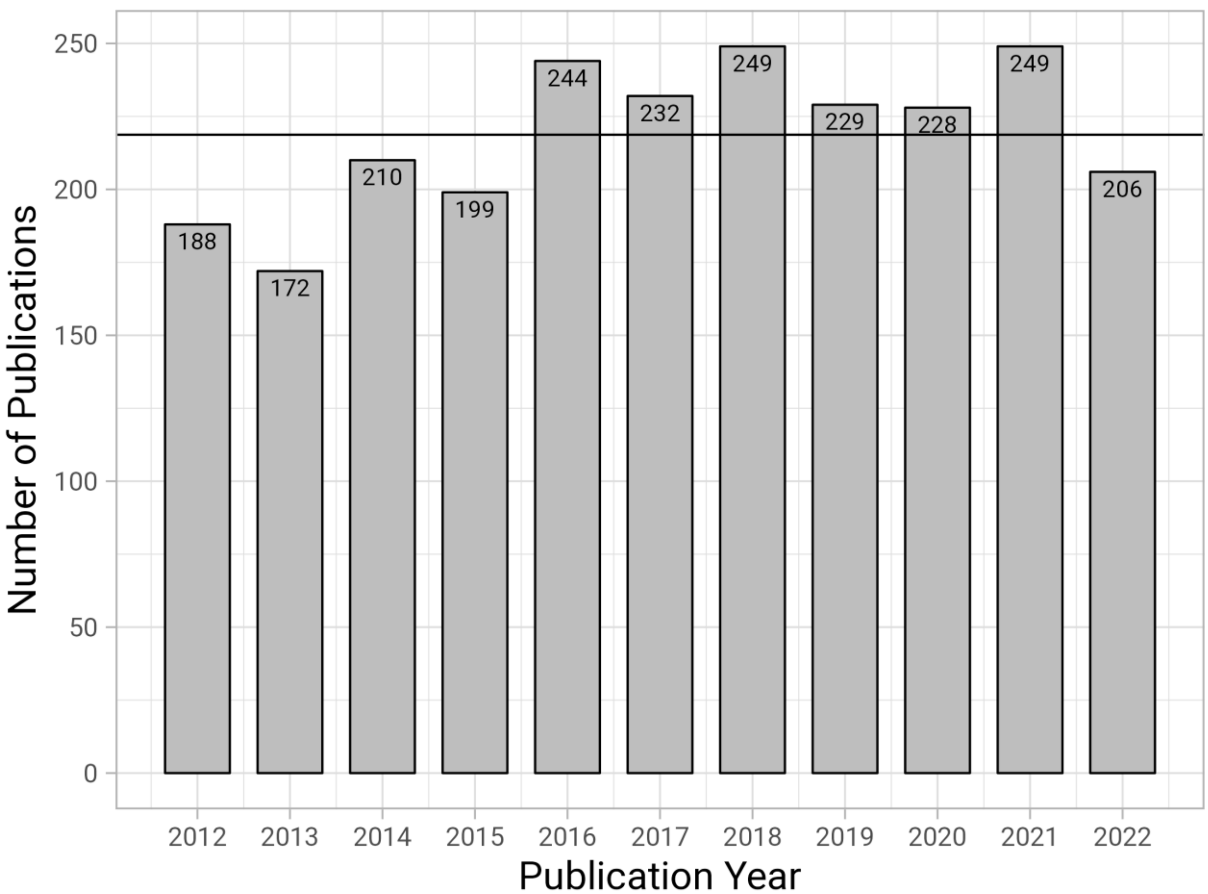


*Figure 1: Publication output of the MPIC per year (articles and reviews) in the years 2012 to 2022 (the black line marks the average of about 219 across all years).*

Table 1 lists the journals in which at least 15 MPIC papers have appeared between 2012 and 2022. The distribution of the MPIC papers across the journals is very strongly skewed: Nearly a quarter of all papers are published in one single journal; it takes only two more to cover a third. To cover a half of all papers it only takes twelve journals, and for two thirds it takes only 31 journals. In total, the MPIC has published in 398 different journals.

*Table 1: Distribution of the MPIC papers (articles and reviews) across journals (limited to the 28 journals having published at least 15 MPIC papers) in the period 2012-2022 (sorted in descending order of the absolute number of papers)*

| Journal | Papers | % Papers | Cumulative % |
|---|---|---|---|
| Atmospheric Chemistry and Physics | 567 | 23.57 | 23.57 |
| Atmospheric Measurement Techniques | 165 | 6.86 | 30.42 |
| Atmospheric Environment | 64 | 2.66 | 33.08 |
| Journal of Geophysical Research - D - Atmospheres | 64 | 2.66 | 35.74 |
| Environmental Science and Technology | 61 | 2.54 | 38.28 |
| Biogeosciences | 53 | 2.20 | 40.48 |
| Geochimica et Cosmochimica Acta | 50 | 2.08 | 42.56 |
| Geophysical Research Letters | 44 | 1.83 | 44.39 |
| Geoscientific Model Development | 42 | 1.75 | 46.13 |
| Science of The Total Environment | 41 | 1.70 | 47.84 |
| Scientific Reports | 35 | 1.45 | 49.29 |
| Meteoritics and Planetary Science | 34 | 1.41 | 50.71 |
| Nature Communications | 31 | 1.29 | 52.00 |
| Earth and Planetary Science Letters | 30 | 1.25 | 53.24 |
| Physical Chemistry, Chemical Physics | 27 | 1.12 | 54.36 |
| Chemical Geology | 26 | 1.08 | 55.44 |
| Geostandards and Geoanalytical Research | 24 | 1.00 | 56.44 |
| Quaternary Science Reviews | 24 | 1.00 | 57.44 |
| Atmosphere | 23 | 0.96 | 58.40 |
| Proceedings of the National Academy of Sciences of the United States of America | 23 | 0.96 | 59.35 |
| Atmospheric Research | 20 | 0.83 | 60.18 |
| Nature Geoscience | 20 | 0.83 | 61.01 |
| Environmental Science and Pollution Research | 17 | 0.71 | 61.72 |
| Science | 17 | 0.71 | 62.43 |
| Bulletin of the American Meteorological Society | 15 | 0.62 | 63.05 |
| Earth System Science Data | 15 | 0.62 | 63.67 |
| Frontiers in Earth Science | 15 | 0.62 | 64.30 |
| Science Advances | 15 | 0.62 | 64.92 |

**Citation impact:** Since the scope and impact of publications vary considerably, the number of publications alone is not sufficient for measuring scholarly success. Neither does it offer a straightforward benchmark for the quality or value of the papers. Indeed, quality may refer to several very distinctive aspects: Elegance, originality, significance or accuracy, but also popularity or even usefulness. Thus, there is no clear definition of quality and no simple way of measuring it. Citations are merely an indication of the attention a paper has received from peers. Nevertheless, numerous studies indicate that a strong correlation exists between impact (measured by citations) and significance or value (measured by rating of peers) (Bornmann, 2011; Diekmann, Naf, and Schubiger, 2012). Given that citations quantify impact as an important aspect of research performance (Martin & Irvine, 1983), they can be recorded and used as proxy data to rate it (provided that the ensembles considered are sufficiently large).

It is a standard approach in bibliometrics to use a minimum citation window of three years after publication (Glänzel, 2008). “After an early (third-year) peak … citedness declines steadily as a function of time since publication, probably reflecting the gradual obsolescence of the article contents (individual articles may of course vary greatly in their citational durability)” (Seglen, 1992, p. 629). In general, the longer the citation window, the more reliable and valid is the measurement of a paper’s total impact. “A long time-span has the additional benefit of reducing random factors and increasing the substantive reasons for being cited” (Research Evaluation and Policy Project, 2005, pp. 20-21).

The standard approach in bibliometrics of using a three-year citation window interferes with the common request of an institutional evaluation to focus on recent years. As a compromise we include in the citation analysis of this report papers from 2020 and accept the reduced reliability and validity of our citation data for this publication year. More details to the time dependence of the MPIC publications’ citations are given in Appendix B.

The MPIC publications of the document types stated (article and review) from 2012 to 2020 (n=1,951), were cited 85,846 times until the end of 2022 (including self-citations by the authors themselves). This leads to an arithmetic average of 44.0 citations per paper (median=21). Appendix C provides information regarding the countries of origin of the papers citing MPIC publications.

**Normalized citation impact:** Different disciplines have different citation habits (i.e., different average numbers of references per paper) resulting in different average citation rates (citations per paper). The average citation rates are varying by a factor of about ten between Mathematics and Molecular Biology & Genetics. Furthermore, the average citation rates seem to depend on the size of the corresponding community and whether the research field is popular or not (Waltman and van Eck, 2013).

For assessing the citation impact with regard to a given scientific community (or for comparing different research units), normalization of the citation data is indispensable. The normalized citation impact can be measured as a quotient of an observed citation rate of an institution and an expected citation rate for the fields of publication (i.e., it compares the performance of an institution to the average performance of the world within specific fields). The expected citation rate is calculated based on a specific WoS subject category (i.e., a journal set) and is defined as the average citation rate for all papers of that document type (articles or reviews), in that subject category, and for the selected publication year. Journals (papers) which are assigned to more than one subject category are considered several times.

Table 2 ranks the major subject categories of the journals in which the MPIC has published its papers in the time period 2012-2020. The subject based observed / expected citation ratios are given as a relative impact measure. A subject based observed / expected citation ratio > 1 means that the citation impact is above the average citation rate of the papers within the corresponding subject category. A subject based observed / expected citation ratio < 1 means that the citation impact is below the average citation rate of the papers within the corresponding subject category.

A VOSviewer visualization (Waltman and van Eck, 2012) of the research activity and citation impact of the MPIC across all subject categories is shown in Appendix D.

*Table 2: Distribution of the* 1,951 *MPIC publications from 2012-2020 with normalized impact values across the relevant subject categories (only the 20 subject categories with more than 15 MPIC papers in total were considered). The subject based observed / expected citation ratios are given as a relative impact measure. Note that many journals are assigned to more than one subject category.*

| Subject category | Number of papers | Citation ratio |
|---|---|---|
| Meteorology & Atmospheric Sciences | 894 | 1.66 |
| Environmental Sciences | 780 | 1.63 |
| Geosciences, Multidisciplinary | 291 | 1.76 |
| Geochemistry & Geophysics | 190 | 1.44 |
| Multidisciplinary Sciences | 125 | 3.37 |
| Ecology | 85 | 1.76 |
| Geography, Physical | 56 | 1.36 |
| Chemistry, Physical | 54 | 1.33 |
| Engineering, Environmental | 52 | 1.26 |
| Physics, Atomic, Molecular & Chemical | 39 | 1.84 |
| Oceanography | 33 | 1.73 |
| Chemistry, Analytical | 30 | 0.89 |
| Paleontology | 30 | 2.33 |
| Chemistry, Multidisciplinary | 27 | 1.13 |
| Astronomy & Astrophysics | 26 | 0.98 |
| Spectroscopy | 21 | 1.35 |
| Forestry | 19 | 1.35 |
| Biochemical Research Methods | 18 | 0.84 |
| Water Resources | 18 | 2.64 |
| Materials Science, Multidisciplinary | 16 | 1.25 |

Figure 2 displays the distribution of the citation ratios for all papers in the 20 WoS subject categories of Table 2 with more than 15 MPIC papers (which amount to 94.0% of all papers of the MPIC with impact values). Three papers have a citation ratio amounting to a high multiple of the respective institute's category mean. The bibliographic data of these most exposed outliers are:

1. *Compilation of Henry's law constants (version 4.0) for water as solvent*. R. Sander (2015), Atmospheric Chemistry and Physics 15 (8), *4399–4981,* DOI 10.5194/acp-15-4399-2015
2. *MIX: a mosaic Asian anthropogenic emission inventory under the international collaboration framework of the MICS-Asia and HTAP*. Li et al. (2017), Atmospheric Chemistry and Physics 17(2), 935–963, DOI 10.5194/acp-17-935-2017

3. *The contribution of outdoor air pollution sources to premature mortality on a global scale.* Lelieveld et al (2015), Nature 525 (7569), 367-371, DOI: 10.1038/nature15371.

If we neglected these three papers in the calculation of the citation ratios, these would cause changes from 1.66 to 1.56 for "Meteorology & Atmospheric Sciences", from 1.63 to 1.52 for "Environmental Sciences ", and from 3.37 to 2.83 for "Multidisciplinary Sciences".

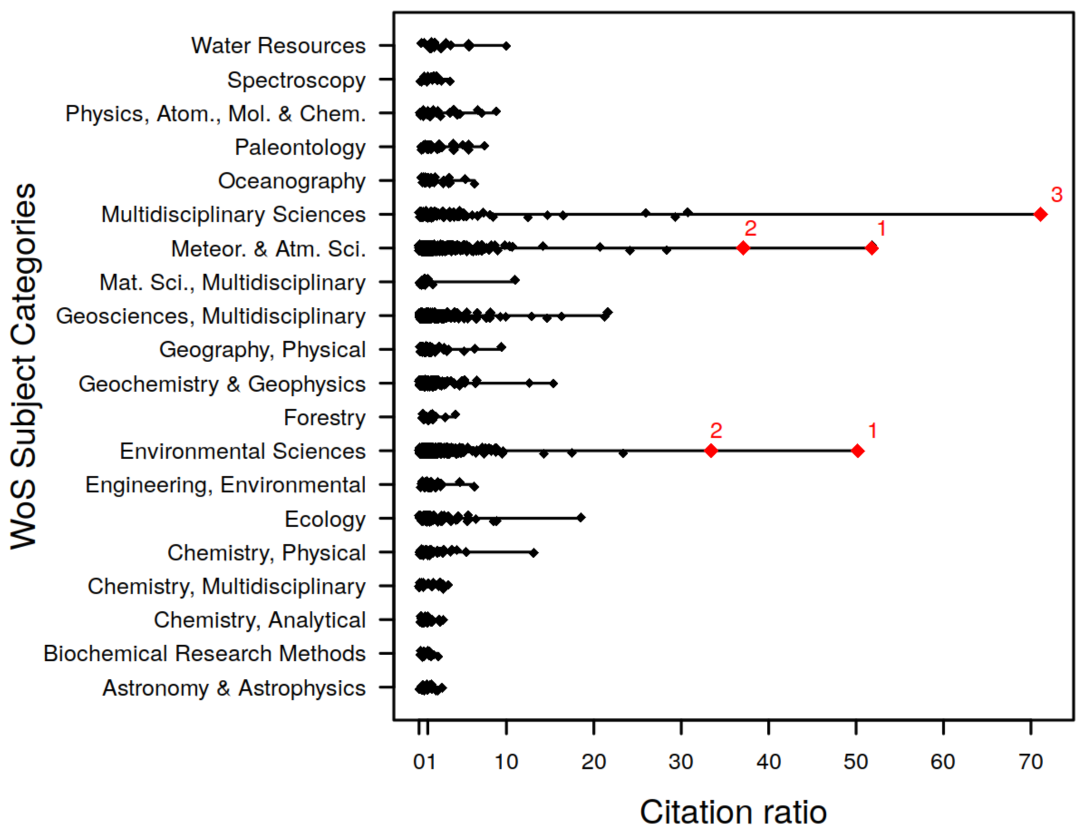


*Figure 2: Distribution of citation ratios across the 20 WoS subject categories from Table 2 in alphabetical order. The three most influential outliers are numbered and colored in red and described in the text body.*

The following rules of thumb formulated by van Raan (2005) – Professor of Quantitative Studies of Science at the Centre for Science and Technology Studies (CWTS) at Leiden University, Leiden, The Netherlands – specifies the interpretation of the category based normalized impact further on: "I regard the internationally standardized impact indicator CPP/FCSm [Table 2: Citation ratio] as the crown indicator. This indicator enables us to observe immediately whether the performance of a research group or institute is significantly *far below* (indicator value < 0.5), *below* (indicator value 0.5–0.8), *about* (0.8–1.2), *above* (1.2–1.5), or *far above* (>1.5) the international impact standard of the field. I stress, however, that for the interpretation of the measured impact value, one has to take into account the aggregation level of the entity under study. The higher the aggregation level, the larger the volume in publications, and the more difficult it is to have an impact significantly above the international level. Based on my long-standing experiences, I can say the following. At the meso-level (e. g., a university, faculty, or large institute with about 500 or more publications per year), a CPP/FCSm value above 1.2 means that the institute's impact as a whole is significantly above the (Western) world average. With a CPP/FCSm value above 1.5 … the institute can be considered to be scientifically strong, with a high probability of finding very good to excellent groups" (pp. 7-8).

Interpreted against the backdrop of these rules of thumb, Table 2 reveals that the MPIC has achieved a subject based observed / expected citation ratio *far above* (citation ratio >1.5) the international standard of the corresponding field in nine of the 20 subject categories with more than 15 MPIC papers, and in seven others *above* the international standard (citation ratio between 1.2 and 1.5). Four other categories are assessed as ranking *about* the international standard (citation ratio between 0.8 and 1.2) and in none of the subject categories of Table 2, the impact has to be considered *below* or *far below* the international standard (citation ratio < 0.8). The above mentioned removal of three outliers in the citation ratio would change the assessment of the impact in none of the subject categories.

**Citation impact according to percentiles:** Until today, it has been customary in evaluative bibliometrics to use the arithmetic mean value to normalize citation data (Waltman, van Eck, van Leeuwen, Visser, and van Raan, 2011). According to the results from Albarrán, Crespo, Ortuño, and Ruiz-Castillo (2011) (and many other studies), the distribution of citations in every subject category is very skewed, however: "The mean is 20 points above the median, while 9-10% of all articles in the upper tail account for about 44% of all citations" (p. 385). The skewed distribution poses the risk that the citation statistics are dominated by a few highly cited papers (Boyack, 2004; Waltman et al., 2012). This is not possible with statistics based on percentiles. Using percentiles to normalize citations can therefore give better comparisons of the impact of publications from different subject areas and years of publication and with different document types than normalization using the arithmetic mean. In the Leiden Manifesto for research metrics, Hicks, Wouters, Waltman, de Rijcke, and Rafols (2015) concluded: "Normalized indicators are required, and the most robust normalization method is based on percentiles" (p. 430).

The percentile provides information about the impact the publication in question has had compared to other publications (in the same subject area and publication year). A percentile is a value below which a certain proportion of observations fall (Bornmann, Mutz, Marx, Schier, and Daniel, 2011; Leydesdorff, Bornmann, Mutz, and Opthof, 2011): The higher the percentile for a publication, the more citations it has received compared to publications in the same subject area and publication year. The percentile for the respective publication is determined using the distribution of the percentile ranks over all publications. For example, a value of 90 means that the publication in question is among the 10% most cited publications; the other 90% of the publications have achieved less impact. A value of 50 represents the median and thus an average citation impact compared to the other publications (from the same subject area and publication year). Since percentiles can be classified into percentile rank classes (e.g., papers belonging to the 10% most cited papers), it is not necessary to use rules of thumb (see above the rules of thumbs of van Raan for the mean-based indicators) for the interpretation of citation impact figures.

InCites – one of the most important customized, web-based research evaluation tools for analyzing institutional productivity and impact (provided by Clarivate Analytics) – calculates percentiles as follows: "The percentile of a publication is determined by creating a citation frequency distribution for all the publications in the same year, subject category and of the same document type (arranging the papers in descending order of citation count), and determining the percentage of papers at each level of citation, i.e., the percentage of papers cited more often than the paper of interest. If a paper has a percentile of value of one, then 99 percent of the papers in the same subject category, year and of the same document type have a citation count that is lower. A percentile indicates how a paper has performed relative to others in its field, year and document type and is therefore a normalized indicator. ... In the case that a paper is assigned to more than one category, the category in which the percentile value is closest to zero is used (i.e. the best performing value)." (InCites, 2019)

Since in a departure from convention low percentile values mean high citation impact (and vice versa), the percentiles received from InCites are called "inverted percentiles". By standardizing the citations using inverted percentiles, we can compare the impact of publications from different subject areas and publication years directly.

Figure 3 shows the result of an impact analysis based on inverted percentiles for the publications (articles and reviews) of the MPIC from 2012 to 2020. The box and dot plot in the figure visualizes the distribution of the inverted percentiles for the different publication years. The box plots consist of a box where the outer borders mark the first quartile (25% of the values) and the third quartile (75% of the values). The red line with the diamond inside the box indicates the median (50% of the values are higher or lower than this value). The position of the median in the box gives an insight into the skewness of the values. The median of all papers is represented by the dashed red line. In addition to the boxes, Figure 3 shows the distribution of the percentiles using a dot plot.

For a facilitated interpretation of the percentile results in Figure 3, Table 3 presents median inverted percentile ranks for all papers from the USA and Germany as well as from the MPIs clustered in the CPT section of the Max Planck Society (CPTS), respectively those clustered in the MPG-internal research field of the MPIC.

*Table 3: Median inverted percentile ranks for the USA, Germany, the CPT section, and the research field compared to the MPIC (publication years 2012-2020)*

| Aggregation unit | Median inverted percentile ranks |
|---|---|
| USA | 41.9 |
| Germany | 43.1 |
| CPTS | 31.5 |
| Research field | 30.5 |
| MPIC | 29.1 |

As shown by the results in Figure 3, the publications of the MPIC have achieved a similar impact each year, which more or less corresponds to the median of all years, med=29.1, based on 1,951 papers. This result points out that the papers the MPI has published between 2012 and 2020 have an impact *clearly above the average* within their subject categories. The comparison of the MPI with the USA and Germany in Table 3 shows that the MPI on average performs significantly better than these countries and also better than the associated research area and the CPT section.

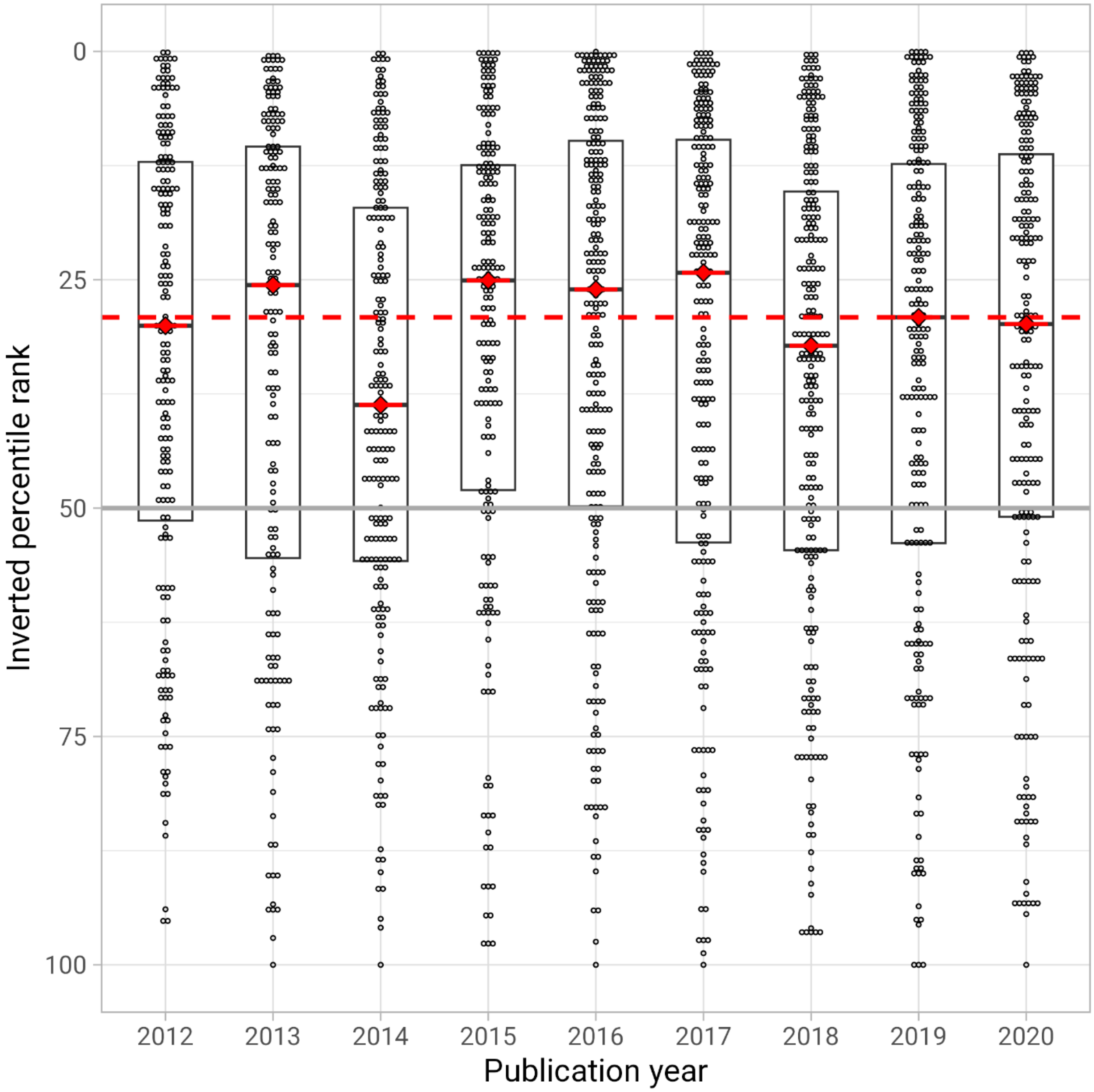


*Figure 3: Distribution of the inverted percentiles for papers (articles and reviews) published by the institute between 2012 and 2020 (*n=1,951*). The lower the inverted percentile of a publication, the higher is its impact in the scientific community. The red dashed line in the graph marks the overall impact of the MPIC* (median=29.1)*. The red bars with the diamonds indicate the median of the institute in the respective years.*

**Top 10% most frequently cited publications:** Since publications that rank among the 10% most frequently cited publications in their field are to be considered as highly cited publications, the percentage of papers from the institute that belong to the top 10% in their field has also been calculated. Statistically, one would expect that 10% of an institution's publications would rank among the 10% of the most cited publications (Bornmann, de Moya Anegón, and Leydesdorff, 2012; Bornmann and Haunschild, 2017; Waltman & Schreiber, 2013). Note that this indicator implies another perspective concerning the citation impact of an institutional unit: The higher the percentage of papers that belong to the top 10%, the higher is its citation impact in the scientific community.

20.6% (3.1%) of the MPIC's papers published between 2012 and 2020 belong to the 10% (1%) most cited papers within their subject categories. The MPI's value of 20.6% highly cited publications (n=401) can be counted as an impressive performance.
In the Leiden Ranking 2023 of universities (http://www.leidenranking.com/) (Waltman, et al., 2012), the top 10% (1%) values are calculated for different four-year time intervals. For the sake of comparison, we take the MPIC's 954 publications between 2016 and 2019 and obtain the values of 21.5% (3.1%) highly cited publications. In the subject field Physical Sciences and Engineering, it is comparable to the world's top universities, such as University of Chicago with 21.5% (3.4%), UC Santa Barbara with 21.2% (3.3%), and Caltech with 20.8% (3.6%), thereby underlining the high quality of the MPI's research. The three top ranked universities with at least 500 publications in that time period are the Stanford with 24.5% (4.4%), Harvard with 23.5% (4.0%), and MIT with 23.1% (4.0%).

Note that the Leiden Ranking uses time slices of four years, each. The time period 2016-2019 was used for comparison although the impact of MPIC was assessed between 2012 and 2020. Furthermore, algorithmically constructed clusters rather than WoS subject categories (as in this study) were used in the Leiden Ranking for normalization of citation impact. Haunschild, Daniels, & Bornmann (2022) have shown that normalized values differ statistically significantly on the level of individual papers if different field classifications are used. However, on the aggregation level of universities both approaches (algorithmically constructed clusters and WoS subject categories) produce impact values which are highly correlated (Perianes-Rodriguez & Ruiz-Castillo, 2015).

**Conclusions**: The bibliometric analysis of the MPIC is based on data retrieved from a bibliometrics database developed and maintained in cooperation with the Max Planck Digital Library (MPDL, Munich) and derived from citation indexes provided by Clarivate Analytics. According to the publication output, this MPI published on average 219 papers (articles and reviews) per year.
Over the years 2012 to 2022, the annual publication output has been slightly increasing. The different metrics used to measure normalized citation impact point out that the MPI has reached a comparatively high impact over the years:

(1) Between 2012 and 2020, the MPIC has published papers which belong on average to the top 29.1% most cited papers within their subject categories. A value of 50% represents the median and thus an average citation impact compared to all publications from the same subject areas and publication years (grey line in Figure 3). A median of 29.1 for the institute (red line in Figure 3) is *clearly above the expected value* of 50 based on the relevant community.

(2) Another indicator implies a different perspective concerning citation impact: About a fifth (20.6%) of the papers published between 2012 and 2020 belong to the 10% most cited papers within their subject categories. That is twice as much as could be expected if the papers were randomly selected. Even more impressive, 3.1% of the paper set belong to the 1% most cited

papers within their subject categories. This is three times as much as could be expected if the papers were randomly selected.

Figure 4 gives a summarizing picture of the time development of the impact that the papers published by the MPIC between 2012 and 2020 have achieved.

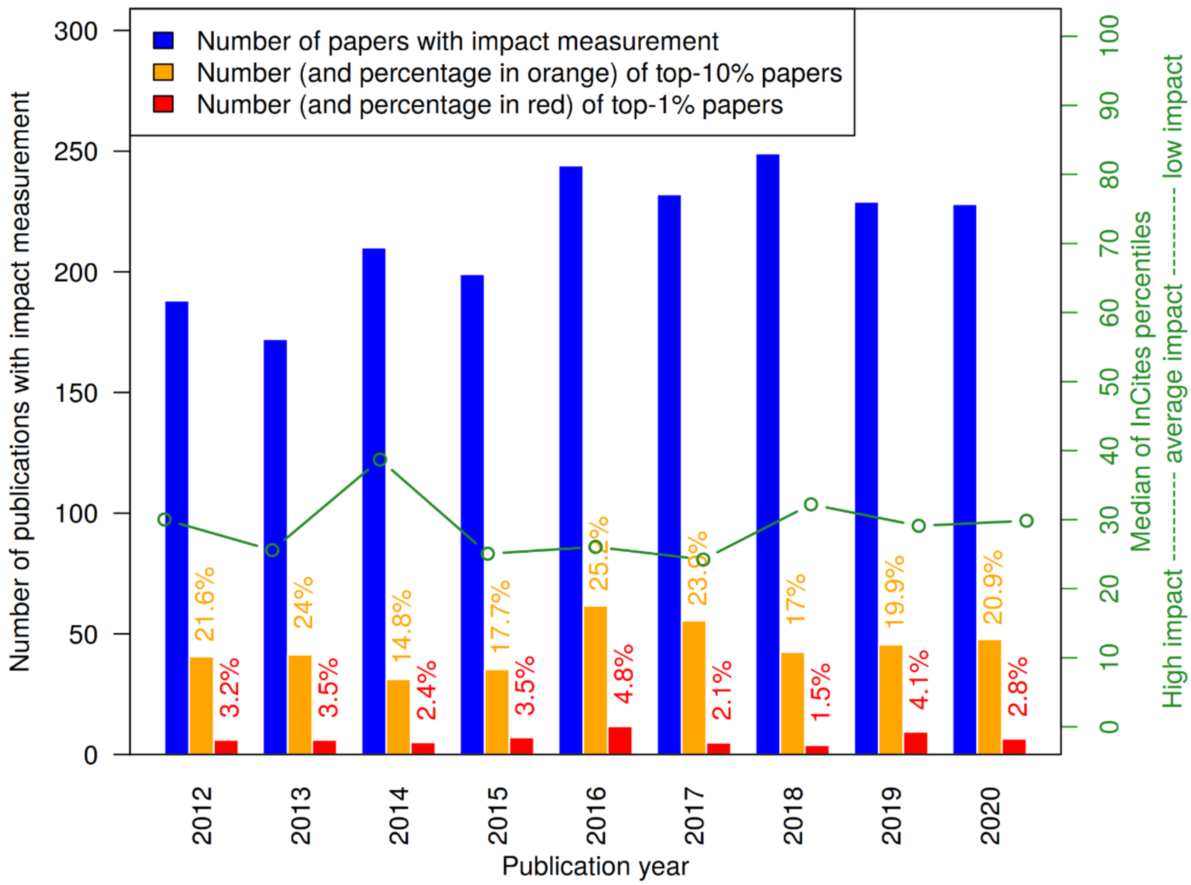


*Figure 4: Summary of the impact information of the papers of the MPIC. An interactive version is available at [https://s.gwdg.de/C8neaA](https://s.gwdg.de/C8neaA).*

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Waltman, L., van Eck, N. J., van Leeuwen, T. N., Visser, M. S., & van Raan, A. F. J. (2011). Towards a new crown indicator: Some theoretical considerations. *Journal of Informetrics, 5*(1), 37-47. DOI: 10.1016/j.joi.2010.08.001.

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## Appendix A:

## Collaborations

The MPIC collaborates with research institutes in different countries. Figure A1 shows a color-coded world map (using a logarithmic scale) according to the amount of co-authorships with the MPIC between 2012 and 2022. Figure A2 shows the same for European countries.

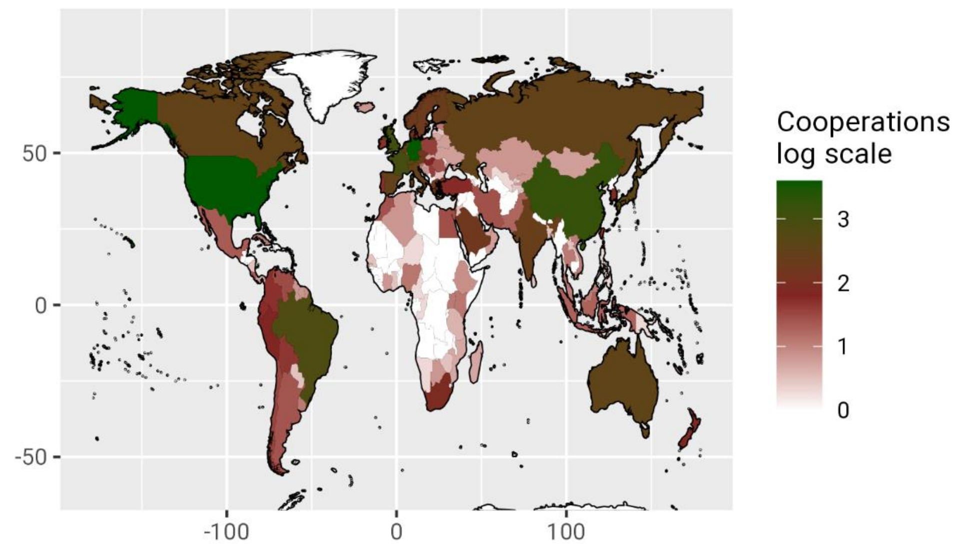


*Figure A1: Color-coded world map according to the amount of co-authorships with the MPIC between 2012 and 2022*

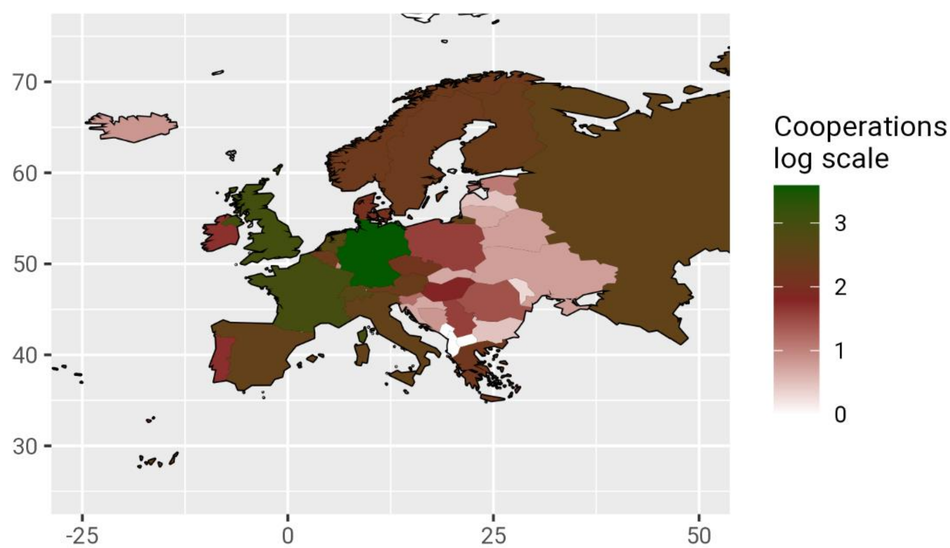


*Figure A2: Color-coded map of Europe according to the amount of co-authorships with the MPIC between 2012 and 2022*

Table A1 lists the number of co-authorships between the MPIC and authors from different countries. MPIC-internal collaborations are not counted.

*Table A1: Number of co-authorships between the MPIC and authors from different countries. Only countries with at least 100 co-authorships are shown. Note that many papers are counted multiple times when the author list contains multiple affiliations.*

| Countries | Papers |
|---|---|
| United States | 3,924 |
| Germany | 3,852 |
| China | 1,611 |
| Great Britain | 1,116 |
| France | 987 |
| Brazil | 708 |
| Netherlands | 532 |
| Switzerland | 495 |
| Japan | 422 |
| Australia | 365 |
| Canada | 321 |
| Russian Federation | 308 |
| Spain | 295 |
| Italy | 292 |
| Cyprus | 279 |
| India | 231 |
| Austria | 226 |
| Finland | 217 |
| Belgium | 201 |
| Sweden | 186 |
| Norway | 180 |
| Greece | 161 |
| Saudi Arabia | 157 |
| Czech Republic | 143 |
| Denmark | 112 |

Figure A3 displays the time development of these collaborations from one five-year-period to another. The red dots denote the percentage of papers in international collaboration from 2012 to 2016, and the blue dots the analogous values for the years from 2018 to 2022. The top 20 countries are shown and the trend is indicated by arrows.

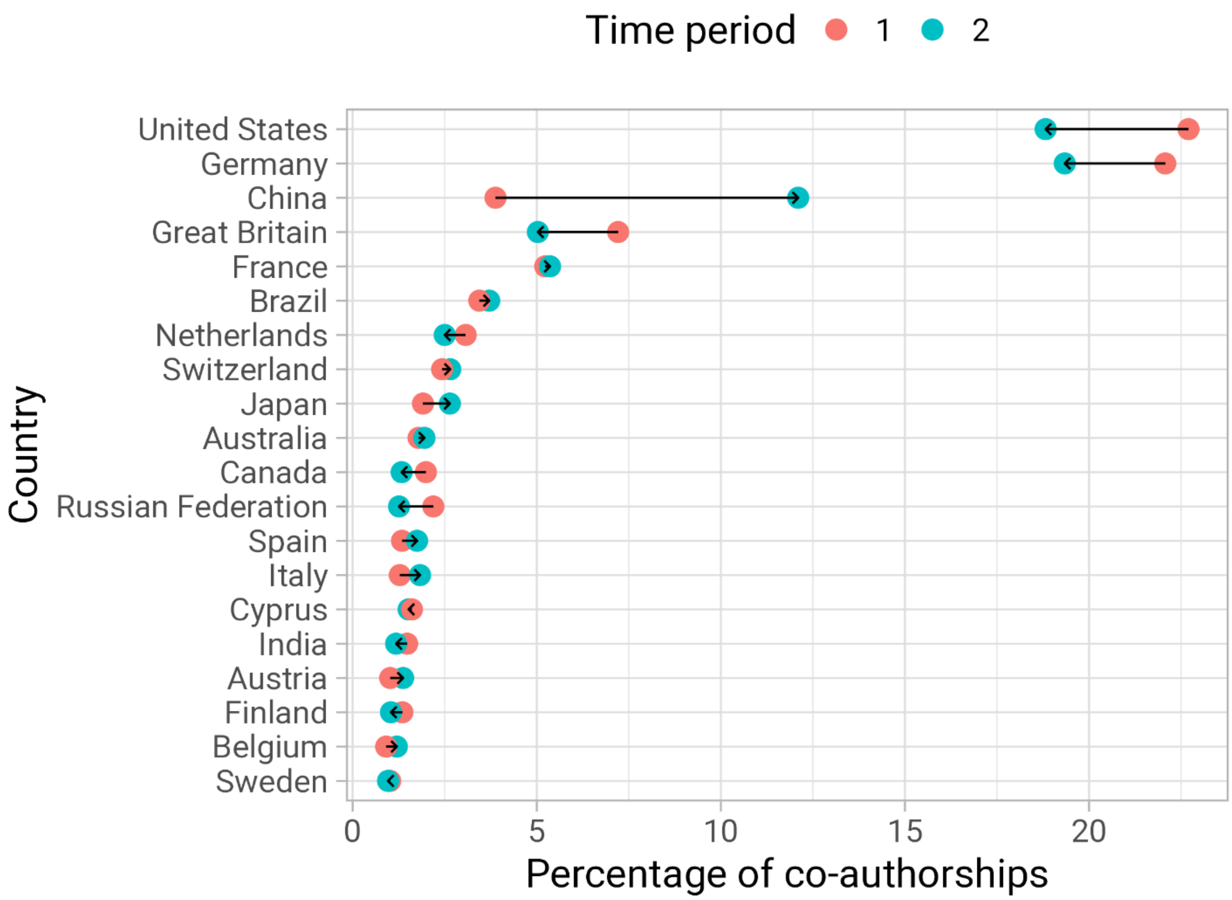


*Figure A3: Comparison of the percentages of international collaborations of the MPIC in the years from 2012 to 2016 and from 2018 to 2022.*

## Appendix B:

## Time Dependence of Citations

A common request in scientific evaluation is a sketch of the performance of the last two years. Unfortunately, citation data cannot give a robust answer to this question.

It is a well-known fact that most publications do not get any citation in the year of their publication. In science we usually find a steep increase followed by a slow decrease in the citation rate. The maximum of the citation rate is centred at about three years after publication but this maximum depends strongly on the scientific field, e.g., in mathematics the scientific response in form of citations is strongly delayed. Figure B1 shows the time dependence of the citation rate of all papers published by the MPIC irrespective of the time period of the analysis in this report. For example, about 6,000 papers cited an MPIC paper within its publication year, and nearly 28,000 papers cited an MPIC paper, that is two or three years old. MPIC papers older than 19 years are cited less often than MPIC papers published in the citing year.

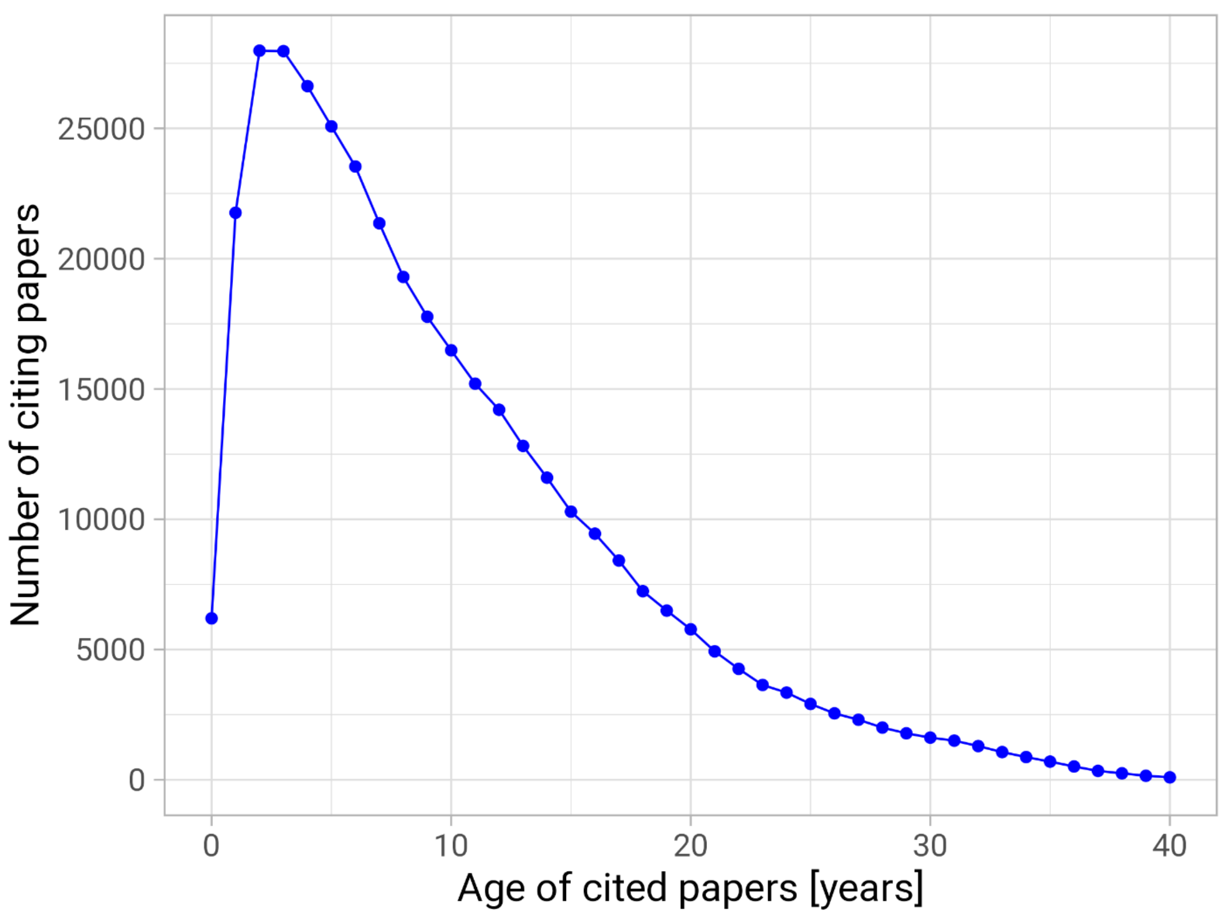


*Figure B1: Time dependence of the citation rate of all papers published by the MPIC*

## Appendix C:

## Citing countries

The MPIC receives citations from publications authored by scientists from research institutes in different countries. Figure C1 shows a color-coded world map (using a logarithmic scale) according to the amount of citations the MPIC has received from a certain country. Figure C2 shows the same for European countries.

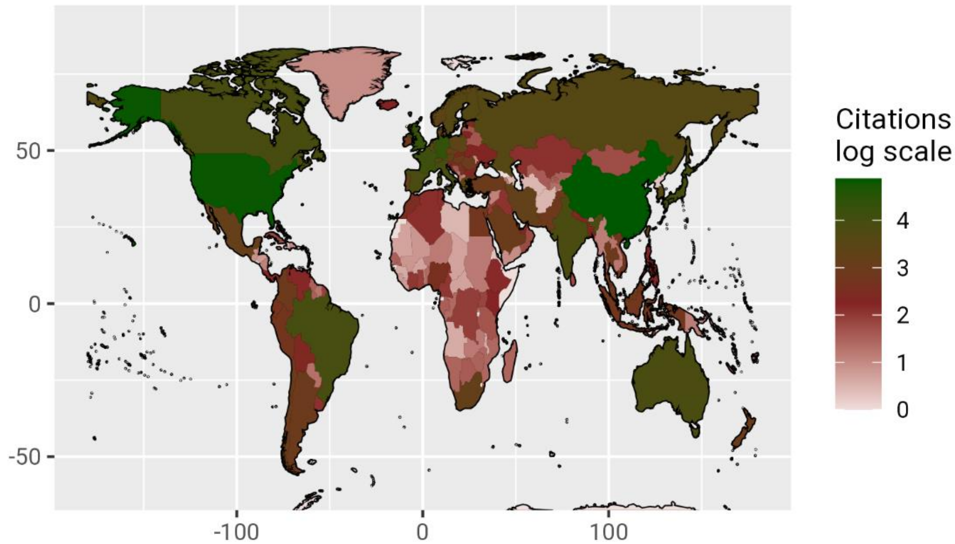


*Figure C1: Color-coded world map according to the amount of citations the MPIC has received between 2012 and 2022*

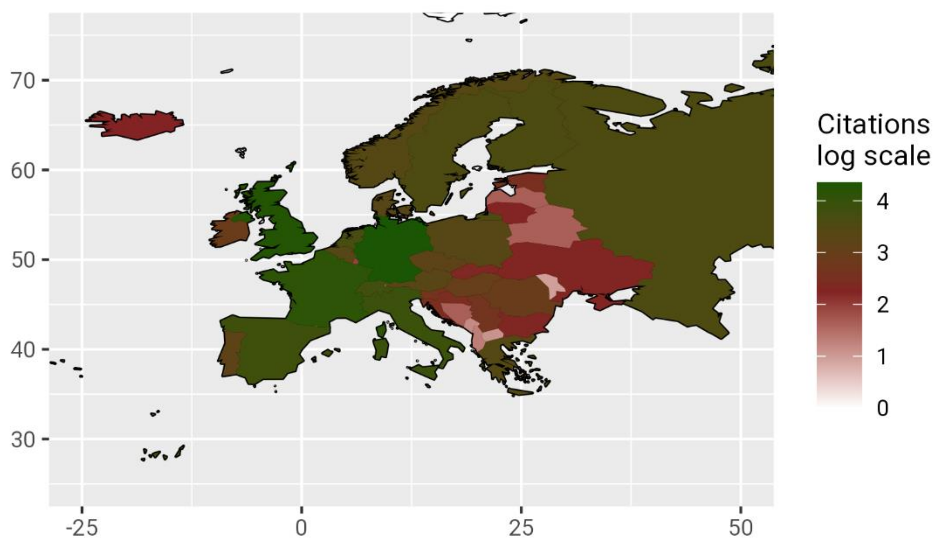


*Figure C2: Color-coded map of Europe according to the amount of citations the MPIC has received between 2012 and 2022*

Table C1 lists the number of papers citing MPIC publications. Self-citations from MPIC papers are not counted.

*Table C1: Number of papers citing publications authored by the MPIC. Only countries with more than 1,000 papers citing MPIC publications are shown. Note that many citing papers are counted multiple times when the author list contains multiple affiliations.*

| Countries | Papers |
|---|---|
| China | 76,154 |
| United States | 68,193 |
| Germany | 22,572 |
| Great Britain | 18,268 |
| France | 13,928 |
| Japan | 9,040 |
| Brazil | 8,647 |
| Italy | 8,613 |
| Canada | 7,992 |
| India | 7,619 |
| Australia | 7,429 |
| Spain | 7,299 |
| Switzerland | 6,201 |
| Netherlands | 4,770 |
| South Korea | 4,347 |
| Finland | 4,110 |
| Sweden | 3,874 |
| Russian Federation | 3,870 |
| Greece | 2,667 |
| Norway | 2,584 |
| Taiwan | 2,428 |
| Poland | 2,358 |
| Belgium | 2,267 |
| Austria | 2,194 |
| Denmark | 2,077 |
| Iran | 1,722 |
| Israel | 1,635 |
| Portugal | 1,578 |
| South Africa | 1,542 |
| Czech Republic | 1,504 |
| Mexico | 1,415 |
| Chile | 1,044 |
| Saudi Arabia | 1,022 |
| New Zealand | 1,020 |

# Appendix D:

## Institutional Profile

An institutional profile shows an institute's research activity and citation impact as overlay visualization. Figure D1 shows the institutional profile of the MPIC.
The institutional profile displays 254 subject categories as nodes, labeled by the corresponding abbreviated names. A list of all short and full names of the WoS subject categories is available at https://s.gwdg.de/AGU8QN. The arrangement of the nodes is based on citation relations between the subject categories considering cited articles and reviews that were published between 2012 and 2020 and citing papers that were published until 2022. The size of the nodes is related to the MPI's activity in these subject categories in comparison to the (WoS) world. In the same manner the colors indicate the impact (by means of citation ratios) the institute has achieved in the subject categories compared to the (WoS) world average.

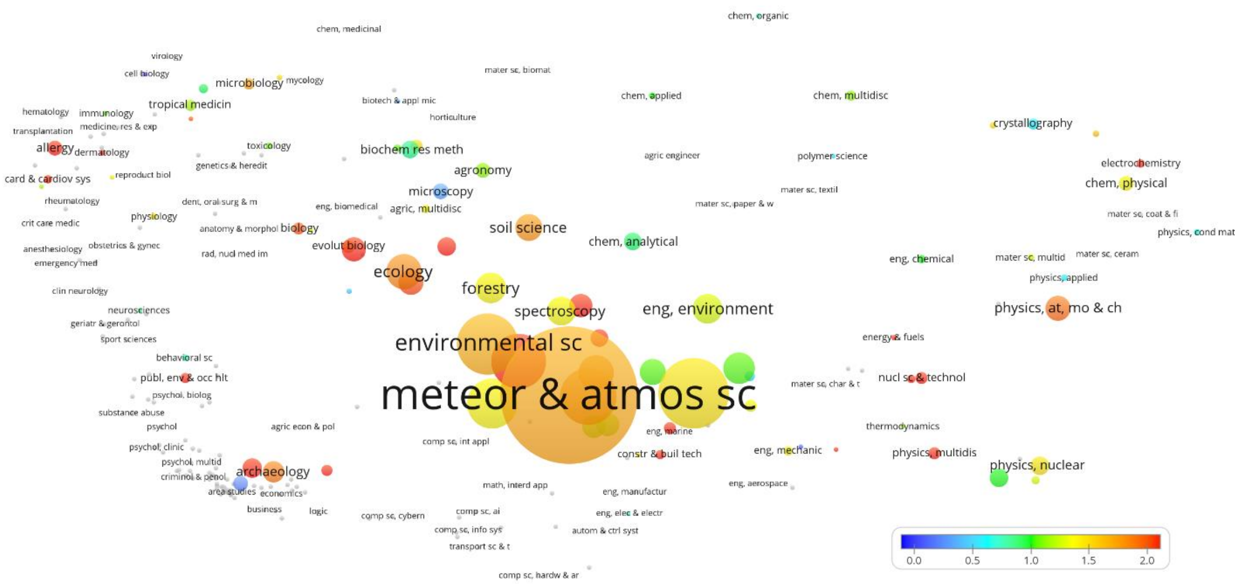


*Figure D1: Institutional profile of the MPIC with respect to the subject categories of its publications from 2012 to 2020. A web-runnable version can be started at: https://s.gwdg.de/Z8bFWB.*


RIO

# Publication Profile: Impact
# Max Planck Institute for Chemistry (Otto Hahn Institute)

Agile Data Report by the Max Planck Digital Library, Big Data Analytics

Munich, 2023–11–17

# Contents

# 1 Introduction

**MPDL.RIO.MPI** is an upcoming service within the Research Information Observatory (RIO) run by the Max Planck Digital Library (MPDL) Big Data Analytics. It strives to enhance the exchange of rich quantitative information on research activities between the MPDL and Max Planck Institutes by providing standard publication profiles as well as publication profile reports specific to individual institutes.

The **standard publication profiles** describe publishing activities of Max Planck Institutes based on data from various sources, institutional repositories, bibliographic databases, and other output metadata services. The data are compiled in a large scale setting encompassing all Max Planck Institutes. Standard reports are produced by highly automated processes and are not fine-tuned for the individual institutes. Depending on the subject domains of the institute the standard representation might not adequately describe the publishing activities.

Besides the standard report, the **MPI-specific publication profiles** can be requested. These reports are fine-tuned to the needs of the individual institutes, for instance including information on the departments and working groups. Preparation is based on the interaction between the institute and the MPDL Big Data Analytics.

Both the standard and the MPI-specific publication profiles exist in two versions. The **output** profile includes statistics and open access categories for the publication output and the **impact** profile additionally includes analyses and comparisons of the citations accumulated by the publications. Since the statistics presented in the impact profile concern sensitive data, the output profile might be suitable to be presented to a broader audience.

The version at hand is an **MPI-specific impact profile** for the **MPI for Chemistry**. Supplementary materials include raw data to all plots and tables which can be used for more customized analyses and visualizations.

**Interpretation** of results should be supported by **informed peers** with a sound understanding of sources of bias, limits of data quality and other caveats to be considered. Consider the **San Francisco Declaration on Research Assessment (DORA)**[1]. See also the appendix for in-depth information on features and constraints from the data sources, our procedures and comments on DORA compliance.

# 2 Data Sources and Methods

## 2.1 Data Sources

Data have been compiled from the following sources:

- Web of Science XML raw data (WoS[2] by Clarivate)
- MPG Publication Repository XML raw data (PuRe[3] by MPG)
- Directory of Open Access Journals (DOAJ[4] by IS4OA)
- Crossref[5] (by PILA)
- Unpaywall[6] (by Our Research)
- Journal Citation Reports (JCR[7] by Clarivate)
- Institutionenkodierung[8] (Competence Network for Bibliometrics by Univ. Bielefeld)
- MPDL.RIO in-house databases for metadata on journals, publishers and institutions (ANDES)

[1] https://sfdora.org/
[2] https://clarivate.com/webofsciencegroup/solutions/web-of-science/
[3] https://pure.mpg.de/
[4] https://doaj.org/
[5] https://www.crossref.org/
[6] https://unpaywall.org/
[7] https://clarivate.com/webofsciencegroup/solutions/journal-citation-reports/
[8] https://www.bibliometrie.info/

**Web of Science** is a bibliographic database with global scope and broad subject coverage. The licensed data set we use includes more than 3 mio articles per year from internationally relevant journals. There are, however, deficiencies with respect to some subject fields relevant for MPG, for instance law and arts history. The subset of Web of Science data licensed for analysis is different from the Web interface available to MPG. Therefore, deviations in the number of publications and citations are to be expected.

**MPG.PuRe** is the institutional publication repository of the Max Planck Society. The data are maintained by the individual Max Planck Institutes. The application (PubMan) is developed and hosted by the Max Planck Digital Library. It includes more than 350 K of publicly available metadata records for a large range of document types predominantly authored by Max Planck scientists.

**DOAJ** includes more than 15 K journals that are pure open access gold and for which metadata are maintained by their publishers. There are, however, some open access gold journals that are not listed.

**Crossref** run by the Publishers International Linking Association Inc. (PILA) provides reference linking by assigning DOIs to scholarly content. Publishers provide metadata to articles via this source. Hence, the data source facilitates the search for metadata about the publisher member, as well as the search for journals corresponding to the given member, and DOIs prefixed with that member ID.

**Unpaywall** is a nonprofit endeavor to make scholarly research more open and accessible. It crawls web pages from more than 50 K locations and identifies more than 20 mio of free scholarly articles. Via the API, metadata on open access status and document location are obtained based on the DOIs in the article records.

**JCR** aggregates the citations metrics of journals included in the Web of Science. It contains the data required to understand the components that index the value and impact of each journal, including the journal impact factor (JIF).

The **Competence Network for Bibliometrics**, funded by the Federal Ministry of Education and Research (BMBF) is a cross-institutional network, focusing on German science metadata. Data from the project "Institutionenkodierung" conducted by the University of Bielefeld are integrated into the RIO data set for standardization of German affiliations found in Web of Science.

**MPDL.RIO in-house authority databases** (ANDES-INST and ANDES-JUNE) are developed and maintained as a platform for thoroughly curated and rich metadata on institutions and journals. They map the information available from external sources to clearly defined entities and hierarchies. Consolidated metadata from external authority databases, bibliographic databases, publisher files, wikipedia, web sites and other sources are provided.

## 2.2 Methods

Data from the external sources are ingested into the MPDL.RIO data lakehouse. Raw data formats (xml, json, csv, txt, xlsx) are converted to json line records which are upload into a PostgreSQL database. The json records are then parsed into relational schemata, cleaned and processed for the specific needs of MPDL.RIO.

The various data sources are then integrated into a **generalized metadata layer** appropriate for quantitative analytics.

The MPDL.RIO in-house authority databases ANDES-INST and ANDES-JUNE are used for standardization and integration of information.

The metadata from bibliographic sources (Web of Science, MPG.PuRe) are fed into a global database of **unique scientific works**. Identical publications within or between the sources are identified either via DOI or pattern comparisons based on various metadata fields.

Basic analytics are run via PL/pgSQL pipelines in the database, any further processing is accomplished with the aid of an in-house **visualization and reporting framework** based on python.

More details about data sources and methods can be found in the Appendix (Section 5).

# 3 Output Results for Max Planck Institute for Chemistry (Otto Hahn Institute)

The reporting period for **long term trends** ranges from **2000-2023**. A shorter **focus period** for recent publications ranges from **2021-2023** and is used for selected statistics. Note that very recent publications might not yet be incorporated in the data sources and thus not be included in this report. Citation counts for very recent publications typically range from zero to a few so citation statistics may not be very robust for those publications. In-depth information on the data sources is given in Section 5.

## 3.1 Output – Comparison between WoS and MPG.PuRe

Several analyses need to be based on publications found in **Web of Science (WoS)**. This currently includes open access categories, subject domains and citation networks.

**Web of Science**, however, has an unbalanced coverage of journals with respect to research domain, internationality and language. Therefore it is crucial to know to what extent WoS is representative for the publication profile of the MPI for Chemistry.

The publication data in **MPG.PuRe** are maintained by the Max Planck institutes and reflect their policies with respect to completeness of output records. Therefore we use MPG.PuRe as a **reference** to judge on the representativity of Web of Science.

We attempt to identify publications that are present in both data sources by extensive matching algorithms based on DOI and other metadata patterns. Despite these efforts undetected duplicates might remain in the data set. For details on these procedures see Section 5 in the Appendix.

Web of Science and MPG.PuRe include different **document types**. In the WoS XML data licensed for analytics we find only document types related to journals, proceedings and series whereas MPG.PuRe additionally includes books, theses, talks and many more. The **base** document types that are of interest in the analysis are article, review, editorial, and letter.

To judge on the representativity of Web of Science, we devide the publications which have a **base** document type in two subsets, **PuRe-only base** if they have only been found in PuRe, and **WoS base** if they have been found either only in WoS or in both WoS and PuRe, see table 1.

If the ratio of the number of publications from subset **PuRe-only base** to the number of publications from **WoS base** is small, it can be assumed that the scientific output of an institute is well reflected in WoS.

All remaining document types (except abstracts) are assigned to the subsets **PuRe-only other** and **WoS other** and are not analyzed in the following sections. Meeting abstracts are not included in any dataset.

For a complete list of WoS document types see table 4.

The number of publications attributed to each subset is shown in Figures 1 and 2 for the MPI for Chemistry and for the Chemistry, Physics and Technology Section (CPTS).

| data source / document type | WoS only **or** WoS & PuRe | PuRe only |
|---|---|---|
| article, review, editorial, letter | **WoS base** | **PuRe-only base** |
| thesis, poster, correction, book, … | **WoS other** | **PuRe-only other** |
| abstract | – | – |

**Table 1** Subsets of document type and data source for futher analysis. Meeting abstracts are not included.

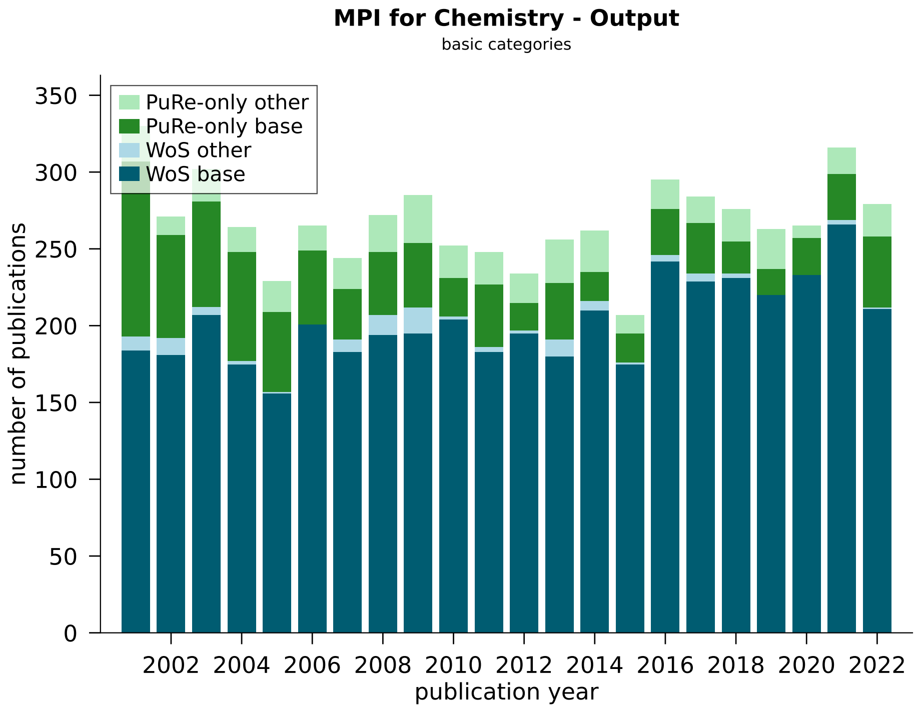


**Figure 1** Number of publications by MPI for Chemistry as a function of publication year. Publications found in WoS (dark and bright blue) are compared to publications found in MPG.PuRe only (dark and bright green). In both cases, the contributions are further split by document type: the darker colors for 'base' document types (article, review, letter and editorial), the brighter colors for 'other' document types.

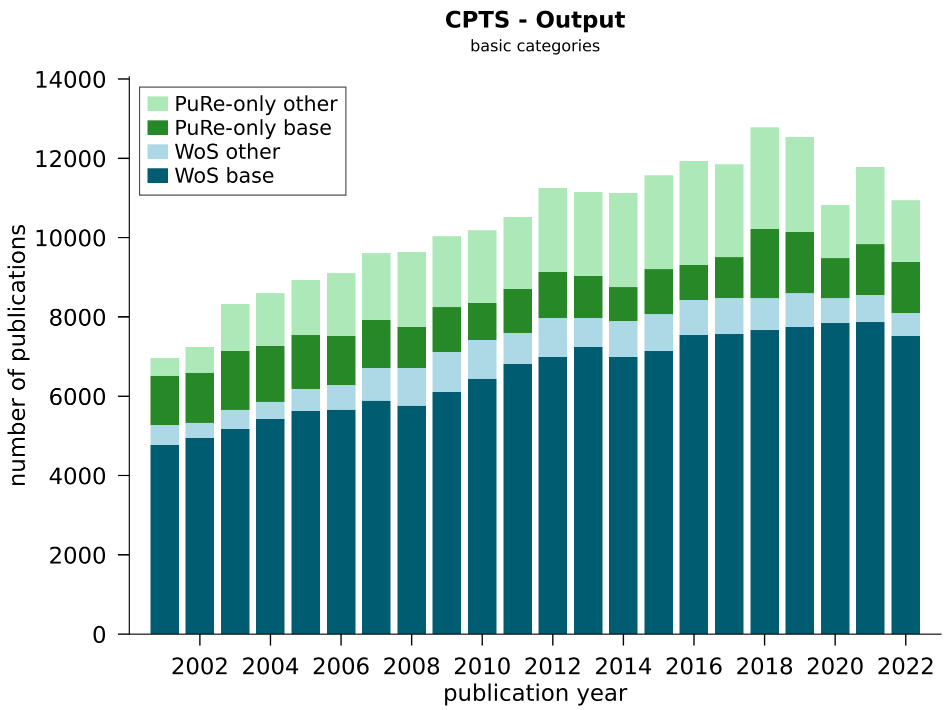


**Figure 2** Number of publications by Chemistry, Physics and Technology Section as a function of publication year. Color coding as in Figure 1.

## 3.2 Journals (WoS base and PuRe-only base)

Figure 3 shows journals in which the MPI for Chemistry published most frequently during the focus time period. The Figures are based on all publications with base document type, i.e., **WoS base** and **PuRe-only base** (see table 1).

Journals are color coded with respect to the **open access status** (see table 2): Journals may be either pure open-access journals or subscription jurnals. In the latter case, it is further distinguished whether there is a transformative agreement with the MPG for this journal or not.

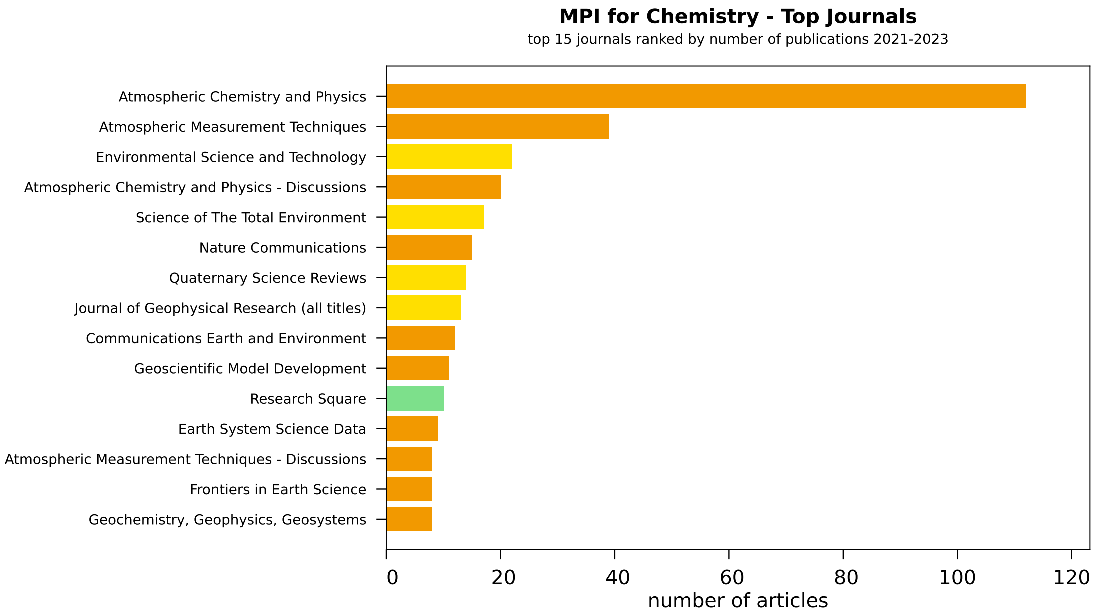


**Figure 3** Journals in which the MPI for Chemistry published most frequently during the selected time span. See table 2 for the color coding. For subscription journals with central transformative agreement (yellow) the starting year of the agreement is shown in parentheses. Note that the total count of publications is shown, which may also include publications before the start date of the agreement and publications from non-MPG corresponding authors.

| color code | access type |
|---|---|
| orange | **gold open access** journal<br>all articles are open access |
| yellow | **subscription journal** with **MPG central transformative agreement**<br>open access is funded by MPG for articles with MPG corresponding authors<br>open access might be funded by other funders for non-MPG corresponding authors<br>standard articles are behind paywall |
| grey | **subscription journal** without MPG central transformative agreement<br>open access might be funded for individual publications by an institute or author<br>standard articles are behind paywall |
| green | **open repository**<br>open repositories like ArXiv or BioRxiv are not covered in Web of Science but can be included in PuRe |

**Table 2** Journal access types

Figure 4 shows the distribution of publications from the MPI for Chemistry which appeared in high impact journals within the selected time period.
The journals in which the institute has published at least one article in the selected time span are ranked with respect to their journal impact factors as indexed in the **Journal Citation Reports (JCR)**[9]. The data is based on the subsets **WoS base** and **Pure-only base** (see table 1).

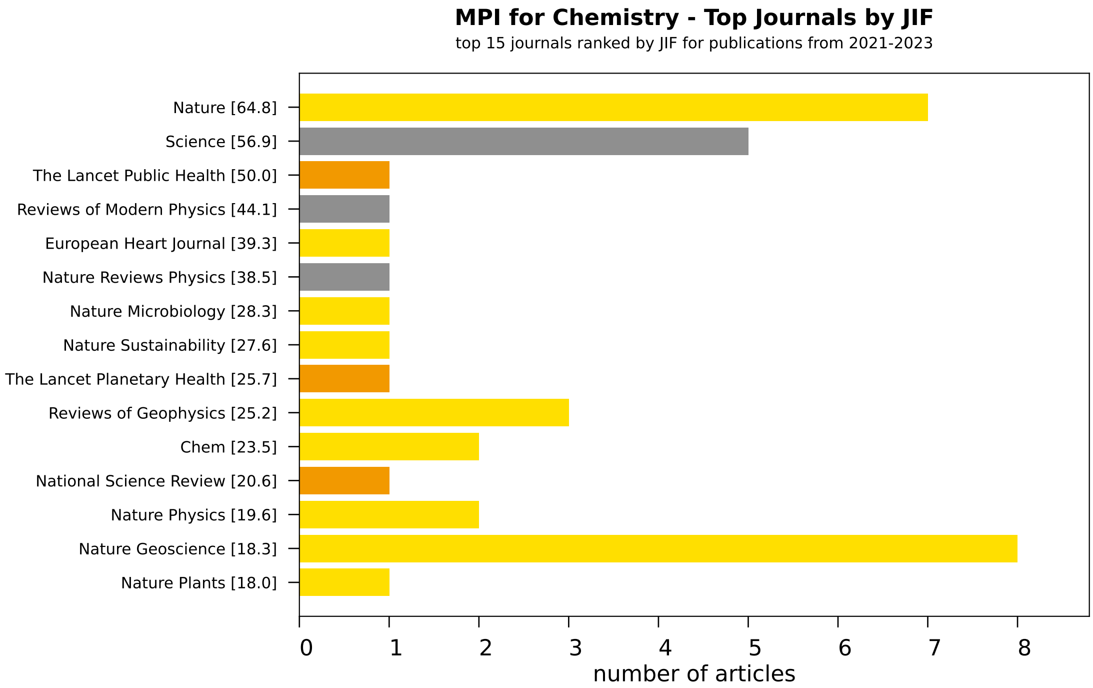


**Figure 4** Journals with the highest journal impact factors in which the MPI for Chemistry has published at least one article in the selected time span. See table 2 for the color coding. The impact factor (JIF) of each journal is shown in brackets.

[9] Note that journal impact factor percentiles provided in the supplementary material are not calculated from the Web of Science raw data, but inserted directly from the JCR raw data from Clarivate.

## 3.3 Journal subject categories (WoS base)

A subject-based analysis of the published articles is provided in Figure 5 which is based on the **Web of Science subject categories**. Note that Clarivate assigns the subjects on the journal level, meaning that all publications from a given journal have the same subject category. One journal can be assigned to multiple subject categories. The data is based on **WoS base**.

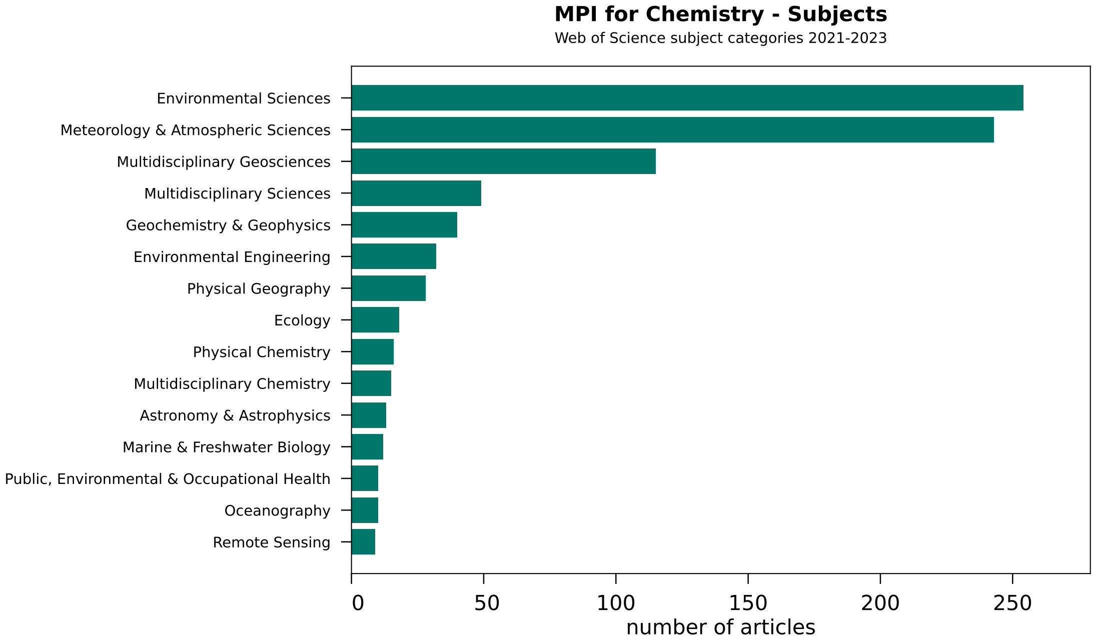


**Figure 5** Most frequent WoS subject categories in which the MPI for Chemistry has published during the selected time span.

## 3.4 Open Access (WoS base)

**Open access information** is derived from Unpaywall, Crossref, DOAJ, and the list of central transformative agreements for the MPG. The data sources are described in detail in the Appendix (Section 5).

Only publications of the subset **WoS base** (see table 1) are considered. Choosing this subset is motivated by the objective to yield shares of open access categories that can be compared between Max Planck institutes. The document types that are deposited in MPG.PuRe and the completeness of the data in general vary considerably between the institutes. Including the subset PuRe-only base would thus lead to results that would hardly be suitable for a comparison to other MPIs or the MPG in total. In addition, in some cases the data from MPG.PuRe lack an entry for a DOI which is crucial for the retrieval of open access information.

Open access categories of publications can be defined with very different approaches. Here we use **four basic levels** of access with an **exclusive assignment** of one category to every publication. If more than one category would apply to a publication we decide based on the sequence

open access gold -> hybrid -> green -> paywall access

The category of a given publication can change with time. Many publishers enable open access at their platform and/or allow the deposit in publication repositories after an **embargo** period of several months. Thus, the share of green open access rises with the age of the publications at the cost of paywall access.

A detailed explanation of our definitions and procedures can be found in the Appendix (Section 6).

Figures 6 and 7 give an overview of open access categories for the MPI for Chemistry and the CPTS. The categories used are:

oa gold (orange): published in a gold open access journal registered in DOAJ

oa hybrid (yellow): published in a subscription journal, but the publisher version of the article is openly accessible from the publisher platform with an open license immediately at the date of publication Usually an article processing charge is paid by the institution of the corresponding author. For MPG this is organized either via central Grundversorgung, the Max Planck institute, or the author

potential oa hybrid (bright yellow): article in a subscription journal, which is probably in the hybrid category but the information available is inconclusive

oa green (green): published in a subscription journal, but an open access version (publisher version and/or preprint, postprint) is available at the publishers platform (usually after an embargo) or in a publication repository

paywall access (gray): published in a subscription journal

oa status unknown (bright gray): no open-access information available, which is often because the DOI of the publication is not known

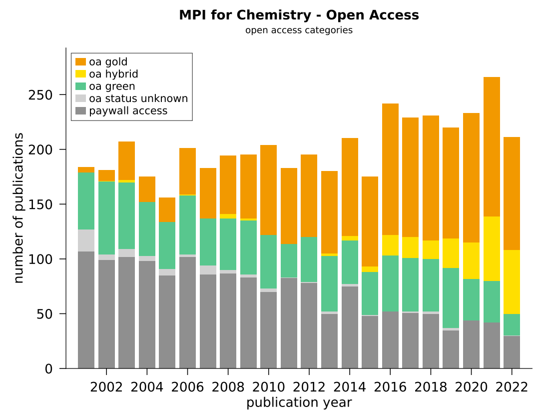


**Figure 6** MPI output by open access categories.

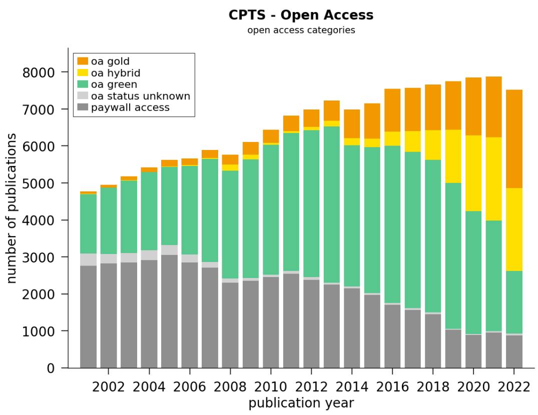


**Figure 7** CPTS output by open access categories.

Figures 8 and 9 show the number of publications available directly on the respective journal website (gold and hybrid categories from Figures 6 and 7). Each journal is assigned to its respective publisher, and the most important publishers (by number of publications) are color-coded and labeled.

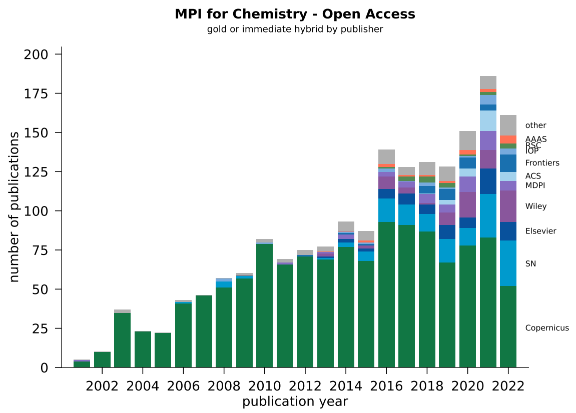


**Figure 8** MPI open access output by publishers.

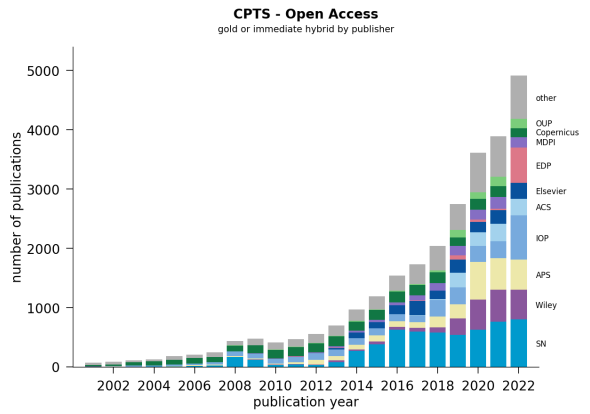


**Figure 9** CPTS open access output by publishers. Top publishers are color coded and labeled.

### 3.5 Output – Collaboration Network (WoS base)

VOSviewer[10] is an open source program from Leiden University. It can be used to interactively construct and visualize bibliometric networks. The nodes of the networks can be selected for analyses on different levels (for example individual publications, authors, or institutes). These nodes can then be connected by different edges (for example based on citations, co-authorship) [1].

Data for the MPI for Chemistry in a format that can be opened with VOSviewer is provided together with this report. All publications that appeared in the **focus period** in **WoS base** are included. The data is based on the Web of Science and enhanced by our standardization of affiliations.

## 4 Impact Results for Max Planck Institute for Chemistry (Otto Hahn Institute)

### 4.1 Citations per Subject Category (WoS base)

Citation metrics indicate the level of attention and scientific discourse intensity that publications have received. They do not measure quality or relevance. See also the **San Francisco Declaration on Research Assessment (DORA)** [11] for caveats when interpreting citation based indicators.

The citation data are compiled from the **Web of Science** raw data. All publications from WoS base are analyzed (see table 1). For counting the number of citations of a publication, all publications that are part of the raw data are considered independently of the document type.

Basic measures of citation frequencies are:

(I) **Total number of citations** to articles published during the selected focus time span.

(II) **Average number of citations** to articles published during the selected focus time span.

Figure 10 compares the number of citations per publication produced by the MPI for Chemistry to the global average number of citations for its top Web of Science subject categories.

[10] https://www.vosviewer.com/
[11] https://sfdora.org/

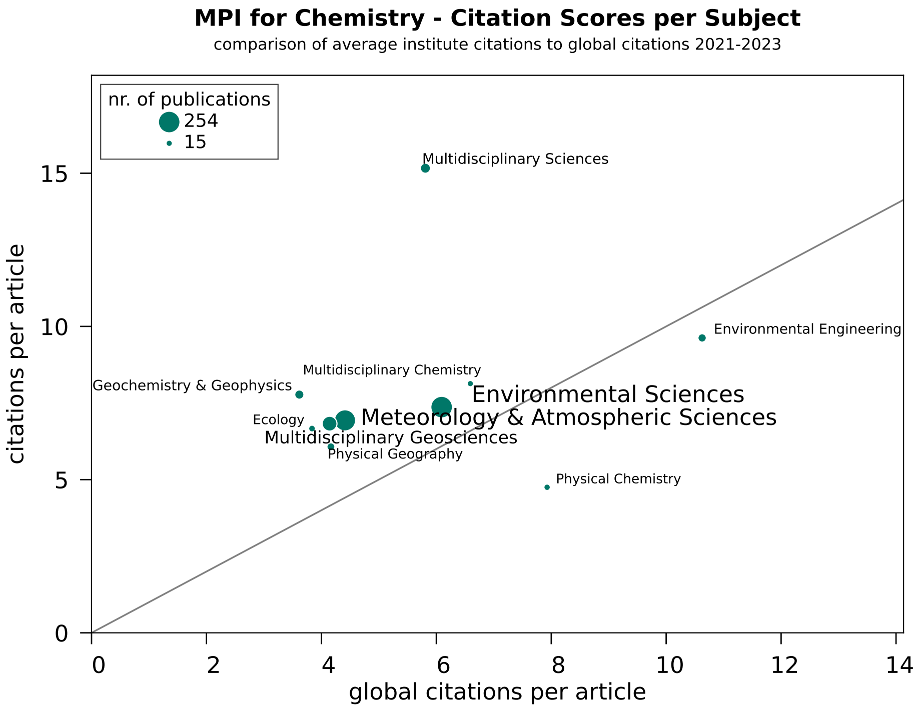


**Figure 10** Citation scores per Web of Science subject category within the selected focus time span. The average number of citations per publication produced by the MPI for Chemistry is compared to the global average number of citations. The 10 fields with the highest number of publications from the institute are shown. Fields with less than 5 publications are not shownThe size of the points represents the number of publications from the institute in each subject field, their number is given in the legend for the largest and smallest of the 10 fields. The solid line in the plot is the diagonal which shows the expected values from the global scores.

## 4.2 Field-normalized Citation Score (WoS base)

Size and publication culture of **scientific communities** have considerable influence on several citation characteristics as are average citation numbers, immediacy of citation, and citation half-lifes.

Citation levels are also related to **document types**. Reviews usually have higher expected values than primary research articles.

The frequency distribution of citations over a set of publications usually is **highly skewed** due to self-inforcing processes (Matthew effect [2]). The average number of citations thus is not robust especially when small data sets are compared.

To correct these influences and achieve a less biased overview, field normalization and ranking procedures are considered.

A **field normalized citation score** for a publication is calculated relative to a reference set of publications published globally in the same subject field, publication year and document type. Several approaches exist:

(III) Mean-based field normalization [3, 4]

(IV) Percentile-based field normalization [5, 6]

(V) Proportion within the top $X$% (top 1%, top 10%) [7][12]

The **mean-based** field normalization approach (III) does not well represent heavily skewed distributions especially for small reference sets. This is overcome with a rank transformation of the reference set. The **percentile-based** field normalization indicators (IV) give the position of a publication within a ranked list.

Several variants for calculating the rank have been suggested which differ in the way they deal with ties (equal citation numbers) and zero values in the reference set. We use a simple approach with a scale from 0 (least citation numbers) to 100 (highest citation numbers). Publications with a percentile above 50 have more citations than half of the publications in the reference set.

Figure 11 shows the distribution of field-normalized percentiles (IV) for the publications of the MPI for Chemistry.

In the supplementary material, the results from a wide range of methods can be found for every publication as well as aggregated values for MPI for Chemistry:

- total number of citations since publication
- average number of citations per year
- number of citations per selected time periods
- relative field normalized citation scores
- average field normalized percentiles
- top 1% and 10% publications

For details on the methods and computations, see Section 7.

[12] The reference sets in [7] are split only by field and publication year, and not by document type. We apply method (V), but split the reference sets by field, publication year, and document type.

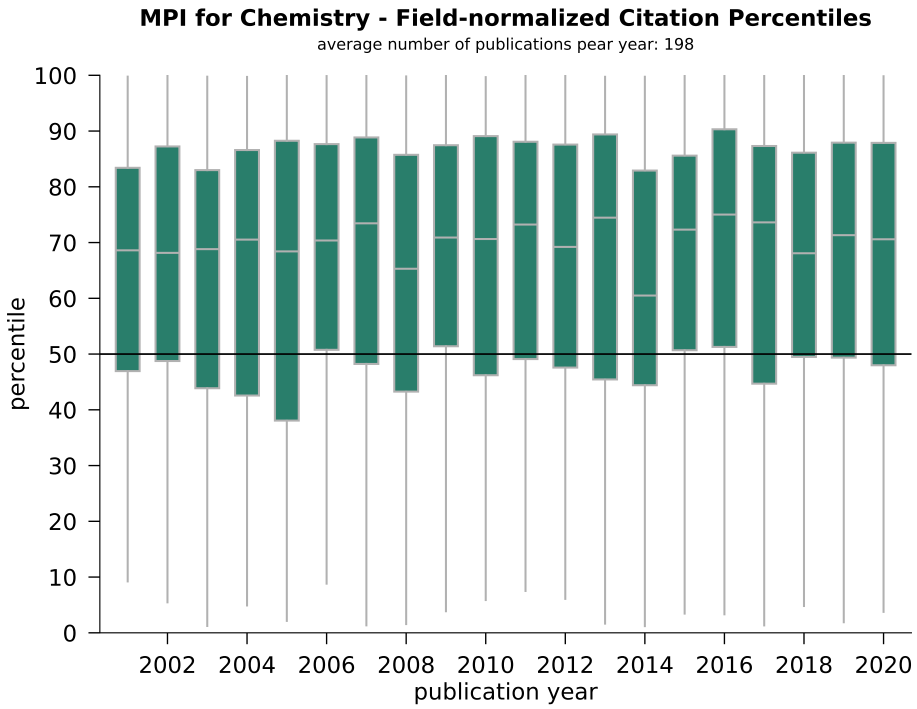


**Figure 11** Field-normalized percentiles for the MPI for Chemistry. Percentiles are calculated for every publication relative to its reference set based on subject field, document type and publication year. The distribution of these percentiles per publication year is shown as a boxplot. (box: first quartile ($Q_1$) to third quartile ($Q_3$); light horizontal line: median; whiskers: all publications that lie within the range $[Q_1 - 1.5(Q_3 - Q_1), Q_3 + 1.5(Q_3 - Q_1)]$, separate dots: outliers). For years with 5 publications or less the publications are shown as individual points. The average number of publications per year where at least one publication was found is given in the subtitle. Boxes with the median above the horizontal line at the 50th percentile indicate that the larger part of the publications of the institute have higher citation ranks than their respective global reference sets. Note that the distribution may be bent towards the 50th percentile for very recent publication years since a large part of the publications, for the institute as well as globally, may have exactly zero citations.

# 5 Appendix – Data Sources

## 5.1 Web of Science (by Clarivate)

The bibliographic data source Web of Science (WoS) is an abstract and citation database provided by Clarivate[13]. WoS covers a broad range of subjects and publishing countries but nevertheless has biases with respect to publication type, internationalization, pervasiveness, impact, and language of the journals in consideration. Table 3 gives an overview of some key characteristics for the database used for this report.

**XML raw data** Whereas general usage of Web of Science is via a web interface on the provider's platform, large scale bibliometric analyses need to be based on inhouse databases that incorporate the raw data that is delivered from Clarivate in XML format. The raw data are licensed by the Competence Network for Bibliometrics[14] (CCB), a German project and consortium funded by the German Federal Ministry of Education and Research (BMBF)[15] under the grant 16WIK2101A. The XML raw data are ingested into a PostgreSQL relational database. Starting from there, MPDL conducts extensive data transformation, cleaning and standardization to make them suitable for further bibliometric analysis.

The Competence Network for Bibliometrics licenses XML data for the basic and proceedings indices of the Web of Science Core Collection[16]. These indices include high impact sources curated by Clarivate along strict criteria. MPDL additonally licenses the Emerging Sources Citation Index (ESCI), which adds more than 7000 high quality journals that do not (yet) fullfill all of these criteria but still are of international interest.

- Basic Indices (1980-)
  - Science Citation Index Expanded (SCI)
  - Social Science Citation Index (SSCI)
  - Arts & Humanities Citation Index (AHCI)
- Conference Proceedings Citation Indexes (1990-)
  - Science (CPCI-S)
  - Social Science & Humanities (CPCI-SSH)
- Emerging Sources Citation Index (ESCI, 2005-) (additionally licensed by MPG)

**XML raw data versus web interface** The MPG licenses several databases offered by Clarivate for the web interface. These include the complete Web of Science Core Collection and other domain-specific resources as are Medline[17], BIOSIS Citation Index[18] and Zoological Record[19]. The indices of the Core Collection which are licensed by the MPG for the web interface but are **not licensed** by the CCB for the **XML raw data** are

- Book Citation Index (BKCI)
- Current Chemical Reactions (CCR)
- Index Chemicus (IC)

Publications from these indices will not appear in the analysis even though they will be visible in the web interface for Max Planck researchers.

**Time lags** There is a delay between the publication of an article and the appearance of the article in the WoS web interface, and an additional delay until the appearance in the XML raw data. Data on recent time intervals therefore need to be interpreted with caution.

**Data quality** Several fields necessary for quantitative analytics are not finally standardized by Clarivate. **Affiliation entries** in the WoS raw data are extremely heterogeneous. For 75 mio articles we find more than 50 mio unique affiliation entries down to the department level. **Journal titles** are largely standardized but still include inconsistencies. **Publisher entries** are very deficient as no special care is taken to unify imprints and follow-up journal titles where the publisher has changed. To improve data quality, we harmonize affiliations, journal titles, and publishers by mapping the data to the MPDL in-house databases on institutions (ANDES INST) and journals (ANDES JUNE) as described in sections 5.6 and 5.7 below.

For the retrieval of data from some sources the DOI is crucial. However, for early publication years the DOI coverage is lower than for more recent publication years (2000 - 73%, 2010 - 85%, 2020 - 95% for the base document types).

[13] https://clarivate.com/webofsciencegroup/
[14] http://www.bibliometrie.info
[15] https://www.bmbf.de
[16] https://clarivate.com/webofsciencegroup/solutions/web-of-science-core-collection/
[17] https://clarivate.com/webofsciencegroup/solutions/webofscience-medline/
[18] https://clarivate.com/webofsciencegroup/solutions/webodscience-biosis-citation-index/
[19] https://clarivate.com/webofsciencegroup/solutions/webofscience-zoological-record/

| | |
|---|---|
| latest data processed (date of delivery by Clarivate) | **2023-03-05** |
| delivery format | XML |
| products licensed | AHCI, SCI, SSCI, CPI, ESCI |
| publication years licensed | 1980 – present |
| number of publications | > 75 000 000 |
| number of references | > 1 600 000 000 |
| number of linked references | > 1 200 000 000 |
| number of publications aligned with JUNE | > 70 000 000 |
| number of affiliations | > 235 000 000 |
| number of affiliations aligned with INST | > 20 000 000 |

**Table 3** Web of Science key characteristics

| document type | base | publications 2020 |
|---|---|---|
| article | x | 2 131 345 |
| abstract | | 237 424 |
| review | x | 173 955 |
| editorial material | x | 149 339 |
| article, early access | x | 116 087 |
| proceedings paper | | 89 442 |
| book review | | 65 377 |
| letter | x | 61 598 |
| correction | | 26 866 |
| article, proceedings paper | x | 23 073 |
| news item | | 14 245 |
| review, early access | x | 8835 |
| biographical-item | | 4731 |
| poetry | | 3727 |
| editorial mat, early access | x | 3420 |
| book review, early access | | 2595 |
| article, data paper | x | 2572 |
| book chapter, review | | 2346 |
| letter, early access | x | 2236 |
| retracted publication | | 1920 |
| art exhibit review | | 1878 |
| article, book chapter | x | 1734 |
| film review | | 1228 |
| record review | | 1120 |
| correction, early access | | 1028 |
| 26 further doc. types | | 2935 |

**Table 4** Web of Science document types as of 2021-04

## 5.2 MPG.PuRe (PubMan by Max Planck Digital Library)

MPG.PuRe is the **pu**blication **re**pository of the Max Planck Society.[20]

The repository's content is generated by the participating Max Planck Institutes and affiliated institutions using the software PubMan. In comparison to other data sources MPG.PuRe contains the widest range of document types, the so-called Genre data sets (such as 'journal articles', 'books', 'films', 'talks', 'thesis', ...). Thus, it represents the publication profile also for institutions that are traditionally not or only sparsely represented in commercial publication data bases like Web of Science.

MPG.PuRe entries are organized in 'collections'. Every institution can maintain multiple of these and thus can manage not only its own publications but e.g. also 'external' or 'non-mpi' collections containing publication data managed with PubMan, but the publications herein are not affiliated with the managing institution. Therefore, we restrict our evaluations only to those collections that are attributable with reasonable certainty as publications of the managing institution.

**Raw data** We take into consideration only those data that are available also via the public web interface. We fetch the raw data as JSON (collection and institution information) and XML (publication information) using MPG.PuRe's REST API[21]. These raw data are subsequently imported into a PostgreSQL relational database and then processed further.

| | |
|---|---|
| delivery format | JSON |
| data fetched on | 2023-03-05 |
| number of publications | > 480 000 |
| number of affiliations | > 830 000 |

**Table 5** MPG.PuRe key characteristics

[20] https://pure.mpg.de/

[21] https://pure.mpg.de/pubman/faces/SearchAndExportPage.jsp

## 5.3 Directory of Open Access Journals (DOAJ by IS4OA)

We use the Directory of Open Access Journals (DOAJ)[22] for identification of gold open access journals. The DOAJ provides a list of 10 K gold open access journal titles along with metadata including publisher information. The content is primarily maintained by the publishers with some extra input via a DOAJ quality assurance team. Completeness and accuracy are therefore heavily depending on the collaboration of the publishers.
For further processing, the journal titles are aligned with the in-house database ANDES JUNE using ISSN and title information. Derived data take into account the OA starting date as journal titles might have changed from subscription to open access during their lifetime. Some prominent examples are the journals transformed in 2014 to gold open access by the Sponsoring Consortium for Open Access Publishing in Particle Physics[23] (SCOAP[3]).
DOAJ constantly adds and sometimes removes journals from its directory. MPDL computes the number of OA Gold articles based on the DOAJ, as a result small oscillations on the number of OA Gold articles should be expected between reports executed with different DOAJ versions. For reproducibility, the download date of the DOAJ is usually included in every report.

| | |
|---|---|
| delivery format | CSV |
| data fetched on | 2022-07-30 |
| number of journal titles | > 16 000 |
| number of publishers | > 4 500 |
| number of journal titles aligned with JUNE | > 13 000 |

**Table 6** DOAJ key characteristics

[22] https://doaj.org/about
[23] https://scoap3.org

## 5.4 Crossref (by PILA)

Another source for our identification of gold open access journals is Crossref[24], run by the Publishers International Linking Association (PILA). Crossref is a non-profit membership organization for scholarly publishing, in which publishers of electronic scholarly content can become members.
As a data source for digital object identifiers (DOIs), we use the Crossref public rest API[25] to access their metadata and fetch the DOIs of publications found in Web of Science and MPG.PuRe. DOIs with minimum publication year of 2015 are then processed into our in-house databases.

| | |
|---|---|
| registered content records | > 120 000 000 |
| member organizations | > 14 000 |
| delivery format | JSON |
| data fetched on | 2022-08-14 |

**Table 7** Crossref key characteristics

Beside providing DOIs for journal content, Crossref provides methods to connect journal articles from different publishers, and so the use of DOIs to link references between articles. Each of 2000 voting member publishers are assigned with a unique DOI prefix. For each registered item in the system, Crossref creates a DOI, incorporating the assigned prefix, and tags it to the article's metadata and the URL where the article resides. With registering and submitting the record to the Crossref database by the publisher, Crossref will register each article DOI and URL in a central DOI directory. This will allow for links to the publisher's content, such that other publishers can retrieve from Crossref the DOIs that link to that content.

[24] https://www.crossref.org/
[25] https://www.crossref.org/services/metadata-retrieval/

## 5.5 Unpaywall (by Our Research)

Unpaywall is a database indexing the open access status for more than 140 mio publications. While also using data from DOAJ and Crossref, the bulk of the license information comes from crawling over 50 000 sources[26] including gold open access journals, hybrid journals, institutional repositories (including MPG.PuRe), and disciplinary repositories[27]. Sources with unclear or possibly dubious copyright status are excluded. Therefore, both ResearchGate and Sci-Hub are not included in the dataset.

Moreover, the database is constantly updated for changes, including: New published articles, new open access articles after embargo periods expire, new open access articles self-archived by authors to repositories, publisher-hosted "Bronze OA" articles (free-to-read but without an open license).

Individual papers can be accessed via a browser plugin. Additionally, the database is integrated into the Web of Science (since 2017) and Scopus (since 2018) web products. However, for large number of articles or more systematic searches, the database can be accessed via an API. For MPDL.RIO we license and ingest the bulk data provided by Unpaywall.

**Open access categories derived from Unpaywall** Unpaywall is an important source to determine open access categories. This source does not provide the “OA color” (Green, Gold, Bronze) of an article, instead it provides the data necessary to derive your own categories.

Unpaywall lists all the publicly available locations where the articles were found along with useful metadata about the location and the article. These fields provide information about whether an article belongs to an gold open access journal or the articles’ journal is in the DOAJ. It also provides the url, the type of location where the article was found (publishers web page, repository, etc.), and information about the access licenses found.

| | |
|---|---|
| data sources | CrossRef, DOAJ, 50 K web locations |
| total number of articles | > 143 000 000 |
| delivery format | JSON |
| data fetched on | 2023-03-05 |

**Table 8** Unpaywall key characteristics

[26] https://api.oadoi.org/data/sources.csv

[27] https://unpaywall.org/sources

## 5.6 MPDL.RIO in-house institution metadata (ANDES INST by MPDL.RIO)

To be able to analyze publication patterns for individual institutions, their affiliation strings are identified in the bibliographic raw data (e.g. Web of Science, Scopus) and aligned to corresponding entries in the in-house database for metadata on institutions. This database serves as a knowledge base on defined institution entities, their metadata and relationships. It is maintained by the MPDL Big Data Analytics Group and includes entries for MPG as well as further institutions included for individual projects of the group. All other German institutions are integrated from the project "Institutionenkodierung" conducted by the University of Bielefeld.

## 5.7 MPDL.RIO in-house journal and publisher metadata (ANDES JUNE by MPDL.RIO)

MPDL.RIO builds and maintains an in-house journal database[28]. This is necessary due to the lack of any resource with complete, accurate and current information on journal metadata, either free or commercial. Most of our data sources include journal information of notoriously bad quality. Even within a given data source many inconsistencies may be expected. Therefore it is not possible to use the primary data for any meaningful quantitative analysis related to journals and publishers.

After 10 years of working with JUNE it indexes more than 100 K unique journal titles. The metadata quality is maintained along the needs of MPG licensing and evaluation activities. Thus, only a subset of some 20 K is checked and updated regularly. Special focus is given to journals listed in WoS basic indices or chosen by Max Planck Scientists for publication.

One of the prominent challenges of maintenance is the follow-up of publishers holding the journal titles. A subset of more than 50 K journal titles is assigned to over 400 explicitly identified publishers. However, only a selection of them is subjected to an in-depth data cleaning and quality assurance. This is usually triggered by MPDL and/or DEAL negotiation requirements.

We developed extensive procedures to harmonize journal titles and assign them to the current publisher. This is notoriously difficult as there is no single reference which provides this information. Constantly changing title names and titles moving from one publisher to another cause significant challenges for accuracy and topicality of the matching process. Within the bounds of our resources, we try to consolidate information from as many sources as possible: title lists from big databases (Web of Science, Scopus, DOAJ) as well as individual title lists from a substantial number of publishers MPDL is interested in.

| | |
|---|---|
| number of identified journals | >100 000 |
| number of identified publishers | >400 |
| number of identified institutions | >6000 |

**Table 9** ANDES JUNE and INST key characteristics

[28] ANDES stands for Authority & Norm Database Entry System, and JUNE is Journal Unique Entries.

# 6 Appendix – Open Access Categories

On the journal level, gold open access from the DOAJ and hybrid status from the transformative agreements of MPDL is stored in the JUNE database together with the starting date and possibly the end date. On the item level, DOI-based information is queried from Crossref and Unpaywall. The full open access information is thus only available if the journal of a publication is identified with an entry in the JUNE and if its has a valid DOI. The conditions for the different categories are tested in the following order:

**oa gold**
In JUNE, the journal has a gold oa status and the publication date is after the date of appearance in the DOAJ; OR the journal is identified as a gold oa journal in Unpaywall.

**oa hybrid**
Crossref indicates a free license with zero delay for the publication; OR in JUNE, the journal has a hybrid oa status, the publication date is between the starting and end dates of the agreement, the reprint affiliation is from MPG and Unpaywall indicates that the publication is openly accessible under a free license at the publisher platform.

**potential oa hybrid**
in JUNE, the journal has a hybrid oa status, the publication date is between the starting and end dates of the agreement, the reprint affiliation is from MPG but there is no information about a free license from Unpaywall or Crossref.

**oa green**
Unpaywall indicates a free version of the publication in a repository, a preprint server or the publisher platform.

**oa status unknown**
No information about the publication is available from Unpaywall.

**paywall access**
in any other case: Unpaywall found no valid oa version for this publication; AND the journal is not resolved in JUNE or has no oa status in JUNE.

# 7 Appendix – Bibliometric Indicators

Bibliometrics covers many aspects to measure the level of attention and interest in publications. Journal impact factors and citation impact are two prominent examples among the various metrics.

The *Journal impact factor* (JIF) of a scientific journal is an index calculated by the Clarivate Journal Citation Reports (JCR). The JIF reflects the average number of citations of articles published in the last two years in a given journal. The JIF percentiles at the item level are taken directly from the JCR. Thus, this type of impact indicates the success level of a publication being published in a journal with high or low rank of impact factors. Based on this index we can calculate the average JIF percentiles to articles published by an institute and its working groups.

The *Citation impact* is the influence of a publication on other academic works and measures its discourse intensity among other publications. Based on this metric, we can calculate citation impact of an institute and its working groups in different ways. The citation impact can be also measured at the item level. Bibliometric analyses for citation impact cover multiple scientific fields. In this regard, bibliometric analyses for an institution rely on bibliometric indicators that provide information on the performance of the institution in different scientific fields. However, scientific fields differ from each other in many aspects, and some of these differences have important implications for analyses. For instance, in some fields, researchers tend to produce more outputs than in other fields. In some fields, researchers focus on publishing articles, while in other fields they are more interested in proceeding papers or books. Also citation patterns from one field to another, and even from one year to another vary substantially.

Given the above-mentioned differences between scientific fields, it is crucial to consider a type of indicators which corrects for these differences. Such an indicator type is referred to *field normalized indicator*, where normalization is considered for:

- research area of the publication (subject)
- publication year
- document type assigned to the publication.

Below we describe several field normalized approaches used for our citation impact analyses.

## 7.1 Citation impact: Field normalized citation score according to Karolinska Institute

A reasonable measure for the citation impact is the field normalized citation score according to the Karolinska Institute (KI) [3, 4]. This score indicates the number of citations compared to the global average of citations to publications in the same subject, document type and publication year, normalized on article level.

**Number of citations**

The *total number of citations* to all publications from an institute during the analyzed time span is given as:

$$C = \sum_{i=1}^{P} c_i, \qquad (1)$$

where $P$ is the number of publications of the institute and $c_i$ is the number of citations to publication $i$.

**Citations per publication**

The ***average number of citations per publication*** of an institute during the analyzed time span is given as:

$$\bar{c} = \frac{1}{P} \sum_{i=1}^{P} c_i. \qquad (2)$$

This score is a measure for the average scientific impact of the institute's publications, but it does not reveal much information with respect to document type, subject area and publication age. For instance, older articles have often collected more citations compared to recent ones. Furthermore, citation rates substantially vary between document types and subject areas.

**Field normalized citation score**

To get a better measure for the scientific impact, the citations of the institute's publications are grouped by different sets. Each set consists of a specific document type, publication year and subject category. The so-called ***item oriented field normalized citation score average*** is defined as:

$$\overline{c}_{\mathrm{f}} = \frac{1}{P} \sum_{i=1}^{P} \frac{1}{N_i} \sum_{j=1}^{N_i} \frac{c_i}{[\overline{\mu}_{\mathrm{f}}]_{ij}}, \tag{3}$$

where $N_i$ is the number of subject areas publication $i$ belongs to and $[\overline{\mu}_{\mathrm{f}}]_{ij}$ is the average citation of the world wide publications corresponding to the same document type, published in the same year as publication $i$ in the subject category $j$.

This score corresponds to the relative number of citations to publications from an institute compared to the global average of citations to publications of the same subject area, document type an publication year. The field normalization is considered on the level of each individual publication. A value $\overline{c}_{\mathrm{f}} = 0.8$ means that the publications of an institute are cited 20% below the average, as well as $\overline{c}_{\mathrm{f}} = 1.5$ corresponds to 50% more citations than on average.

For other mean-based normalization methods, see for example [8], for source normalized citation scores see for example [9].

## 7.2 Citation impact: Percentile-based indicator according to Hazen

The ***percentile rank index*** (PRI) specifies the citation rank of publications of an institute among all publications of the same document type, subject and publication year. For instance, a publication is assigned to the 90th percentile, if 90% of all other publications in the same set received fewer citations.[29] The 50th percentile is identical with the median, indicating the average impact.[30] In this section we consider the percentile ranking index based on Hazen's approach [5, 6].

The publications from an institute are grouped by their publication years, document types and subject categories into different sets. Let's consider a certain set. The number of all publications in that set is denoted as $P$. All publications in the set can be ranked based on their number of citations. Let $r_i$ denote the rank of publication $i$ with respect to its number of citations. If all publications have distinct numbers of citations, the rank of publication $i$ simply holds $r_i = i$. For $n$ publications with the same number of citations, the rank has to be calculated as:

$$r_i = \frac{1}{n} \sum_{j=i_k}^{i_k+n} j, \tag{4}$$

where $i_k$ is the lowest index of the publications with equal number of citations. I.e. ranks of publications with equal number of citations are assigned with the average rank as the arithmetic mean (which can be non-integer). The total average rank (which is the rank of the median) can be computed from the minimum and maximum ranks:

$$r_{\text{avg}} = (i_{r_{\text{min}}} + i_{r_{\text{max}}})/2. \tag{5}$$

The percentile $p_i$ of each publication $i$ in the set is calculated as:

$$p_i = [(r_i - a)/P] * 100, \tag{6}$$

where $a = 0.5$ is the so-called *Hazen coefficient* [6]. The center position of the citation distribution equals the 50th percentile (i.e. the *median*). The property of the median is that 50% of the publications have fewer (or equal) number of citations compared the median, and 50% of the publications have more (or equal) citations.

### Example

Let's assume a simple set with odd number of publications $P = 15$. In table 10 the 15 example publications are ranked with respect to their hypothetic numbers of citations (calculated based on equation 4). For instance, the rank of publication 3 with the same number of citation as publication 4 is: $r_3 = (3 + 4)/2 = 3.5$. The median is on the publication number: $r_8 = r_{\text{avg}} = (r_{\text{min}} + r_{\text{max}})/2 = (15 + 1)/2 = 8$ and corresponds to 50th-percentile. For determining the percentile of $r_{15}$, let us examine equation 6: $p_{15} = (r_{15} - 0.5)/15 * 100 = 14.5/15 * 100 = 96.67$. As several publications in the selected set have equal number of citations, they result in the same values of percentiles, known as **ties**.

[29] Note that PRI can also be used for ranking articles at the journal level (see for example [10]).

[30] Keep in mind that *mean* or *average* usually refers to the arithmetic mean, which differs from the median.

| $i$ | $c_i$ | $r_i$ | $p_i/100$ |
|---|---|---|---|
| 15 | 22 | 15 | 0.97 |
| 14 | 10 | 14 | 0.90 |
| 13 | 8 | 13 | 0.83 |
| 12 | 5 | 11.5 | 0.73 |
| 11 | 5 | 11.5 | 0.73 |
| 10 | 4 | 9.5 | 0.60 |
| 9 | 4 | 9.5 | 0.60 |
| 8 | 3 | 8 | 0.50 |
| 7 | 2 | 6 | 0.37 |
| 6 | 2 | 6 | 0.37 |
| 5 | 2 | 6 | 0.37 |
| 4 | 1 | 3.5 | 0.20 |
| 3 | 1 | 3.5 | 0.20 |
| 2 | 0 | 1.5 | 0.07 |
| 1 | 0 | 1.5 | 0.07 |

**Table 10** Calculated ranks and percentiles for a sample set with 15 articles. Publications (with index $i$) are sorted in descending order by their number of citations $c_i$. The rank $r_i$ denotes the position of each publication in the set. Percentiles $p_i$ are calculated according to the Hazen approach with coefficient $a = 0.5$ and rounded to their second decimals.

## 7.3 Citation impact: Proportion of frequently cited publications according to Waltman and Schreiber

A straight-forward percentile-based bibliometric indicator is the ***proportion of frequently cited publications*** $PP_{top\ x\%}$ i.e. the proportion of publications that belong to the top $x$% most frequently cited of their fields. The calculation of percentile-based indicators suffers from difficulties caused by the discrete nature of citation distributions and equal number of citations of several publications. Waltman and Schreiber [7] introduced a method for calculation of percentile-based indicators, that deals with these difficulties in a more satisfactory way than previous methods.

To illustrate the problem, let us consider a set of 105 publications: 70 without citations, 20 with 5 citations, 10 with 20 citations, and five with 30 citations each. The question, which publications belong to the top 10% is not so easy to answer in that case. Obviously, the five publications with 30 citations belong to the top 10%, but if we also consider the 10 publications with 20 citations to be in the top 10, we have $15/105 * 100 = 14.3\%$ of the publications in the top 10%, what is inconsistent. Also excluding the publications with 10 citations is a bad solution, because then only $5/105 = 4.76\%$ of the publications is in the top 10%. A fair way to handle this, is to consider the publications with a number of citations at the threshold value (in this case 20 citations) with a correction weight such that those weighted publications at the threshold plus those above the threshold correspond to 10% of the total number of publications.

#### Methodology

The above considerations can be written in a more formal way: Let $x$ be the percentage we want to consider in the top $x$%, $n_t(x)$ denotes the number of publications with a citation score exactly at the threshold (depending on $x$), and $n_a(x)$ be the number of publications with a citation score above the threshold. The total number of publications is $P$, and the correction factor is $F$. The number of publications in the top $x$% is denoted as $P_{top\ x\%}$ and holds:

$$P_{top\ x\%} = P \cdot \frac{x}{100} = n_a(x) + F \cdot n_t(x). \tag{7}$$

Rearrangement of Eq. 7 gives the correction factor $F$ for the threshold publication as

$$F = \left(\frac{P \cdot x}{100} - n_a(x)\right) \cdot \frac{1}{n_t(x)}. \tag{8}$$

In the case of top 10%, it is $x = 10$, in the case of top 1%, $x = 1$. The thresholds for 1% and 10% are usually different.

#### Example

In the example above, we have a total number of publications of $P = 105$. In the case of top 10% (i.e. $x = 10$), we have a threshold value of 20 citations, and a number $n_t = 10$ of publications with exactly that threshold value as number of citations. The number of publications with citations above the threshold is $n_a = 5$. We get a correction factor of

$$F = \left(\frac{105 \cdot 10}{100} - 5\right) \cdot \frac{1}{10} = 0.55$$

for the 10 publications with 20 citations.

In the case of top 1% (i.e. $x = 1$) we have a different threshold value of 30 citations, and a number $n_t = 5$ of publications with exactly that threshold value as number of citations. The number of publications with citations above the threshold is $n_a = 0$. We get a correction factor of

$$F = \left(\frac{105 \cdot 1}{100} - 0\right) \cdot \frac{1}{5} = 0.21$$

for the 5 publications with 30 citations.

#### Meaning on institute level

If an institute has 12 publications (in the set of the 105), 1 with 30 citations, 3 with 20 citations, 3 with 5 citations and 5 without citations, we get for the proportion of frequently cited publications:

$$PP_{top\ 1\%} = \frac{(1 \cdot 0.21)}{12} = 0.0175 \approx 1.8\,\%$$
$$PP_{top\ 10\%} = \frac{(1 + 3 \cdot 0.55)}{12} = 0.2208 \approx 22\,\%$$
$$PP_{top\ 20\%} = \frac{(1 + 3 + 3 \cdot 0.60)}{12} = 0.4833 \approx 48\,\%$$

This institute has a proportion of 1.8% of it's publications in the top 1%, 22.1% of it's publications in the top 10% and 48.3% in the top 20% of the comparison set of 105 publications from above.

## 7.4 Altmetric Attention Score

The Altmetric Attention Score addresses the level of interest and attention that publications have received among research communities and in the public media. We fetch the data from the service provider Altmetric. Altmetric tracks online sources for mentions of research outputs. Some of these attention sources are: policy documents, mainstream media and news, blogs, patent citations, Wikipedia, social media as Youtube, Twitter (public tweets, quoted tweets and retweets only, no favorites) and Facebook (posts on a curated list of public pages only, no individual page, no group posts and no likes). To identify how much and what type of attention a publication has received, a graphic visualization of the Altmetric data in the shape of a 'donut' is provided for each publication. Different colors of the donuts represent the volume and the type of attention from different online sources. The attention scores written inside the donuts represent the weighted approximation of all the attention. The attention score for a publication indicates the amount of media attention that it has received.

#### Methodology

For each publication from the institute during the selected time span and base document type, the mention counts from various media sources, overall attention score and detailed information are provided in a badge. The attention score is calculated as *weighted approximation* of all the attention, picked up for a publication (i.e. some data points contribute more than others).

For example, the default attention weight of the media source 'News' is 8, whereas 'Twitter' is weighted as 1 and 'Youtube' as 0.25[31]. The scoring algorithm is determined and executed by Altmetric. Note that the attention can be both positive and negative. Thus, the given score is not a measure of the quality of the research, or the researcher.

Furthermore, it is possible that an attention score of a publication decreases from its previous score. This can happen due to the following reasons:

- Post deletion: thus, the mention from the relevant source is removed from the Altmetric database.
- Modification on weight approximation of biased tweets: thus, weight of those tweets will contribute less to the score than tweets from unbiased accounts.
- Optimizations to the scoring algorithm by Altmetric: thus, all articles in their database are re-scored.

The validity of the attention scores as a complementary benchmark and their accuracy have been questioned by many recent studies. In [11], authors have investigated whether the attention score correlates with the quality of publications. The correlation between citation metrics and attention score has been examined by many other recent studies (see for example [12]). As a result, the attention score alone is not sufficient for quantifying the scientific impact and thus cannot replace the citation-based metrics. Nonetheless, Altmetric can provide qualitative data as a supplement alongside the citation indicators.

[31]For information on default weightings from all attention sources, visit https://help.altmetric.com/support/solutions/articles/6000233311-how-is-the-altmetric-attention-score-calculated-

# 8 Appendix – Declaration on Research Assessment (DORA)

https://sfdora.org

**General Recommendation**

1. Do not use journal-based metrics, such as Journal Impact Factors (JIF[32]), as a surrogate measure of the quality of individual research articles, to assess an individual scientist's contributions, or in hiring, promotion, or funding decisions.

➔ we deliver a huge range of metadata and metrics at the individual article level and explicitly discourage the use of JIFs for the assessment of researchers or institutions

➔ we add the JIF for the judgment of publication channels at the journal level

➔ we add the JIF at article level for convenience - unfortunately it is a mandatory measure for grant applications in some domains (eg medicine)

**For Funding Agencies**

2. Be explicit about the criteria used in evaluating the scientific productivity of grant applicants and clearly highlight, especially for early-stage investigators, that the scientific content of a paper is much more important than publication metrics or the identity of the journal in which it was published.

➔ we explicitly fortify our clients to use data for informed peer review not to replace peer review

➔ we provide a wide range of metadata thus reducing the weight of any one-dimensional ranking metric

3. For the purposes of research assessment, consider the value and impact of all research outputs (including datasets and software) in addition to research publications, and consider a broad range of impact measures including qualitative indicators of research impact, such as influence on policy and practice.

➔ we provide a largely complete output list (any type) for MPG authors by including MPG.PuRe

➔ we include many different impact measures: several citation statistics, altmetrics, network parameters, ...

➔ we include strategic aspects such as open access status

**For Institutions**

4. Be explicit about the criteria used to reach hiring, tenure, and promotion decisions, clearly highlighting, especially for early-stage investigators, that the scientific content of a paper is much more important than publication metrics or the identity of the journal in which it was published.

➔ see 2.

5. For the purposes of research assessment, consider the value and impact of all research outputs (including datasets and software) in addition to research publications, and consider a broad range of impact measures including qualitative indicators of research impact, such as influence on policy and practice.

➔ see 3.

**For Publishers**

6. Greatly reduce emphasis on the journal impact factor as a promotional tool, ideally by ceasing to promote the impact factor or by presenting the metric in the context of a variety of journal-based metrics (e.g., 5-year impact factor, EigenFactor[33], SCImago[34], h-index, editorial and publication times, etc.) that provide a richer view of journal performance.

➔ we are dedicated to analyze the portfolio of publishers for other criteria than the JIF

➔ one of our main activities is to analyze open access characteristics of journals

7. Make available a range of article-level metrics to encourage a shift toward assessment based on the scientific content of an article rather than publication metrics of the journal in which it was published.

➔ we decidedly encourage publishers to deliver article based measures (this would also be a great help for statistics supporting license negotiations)

8. Encourage responsible authorship practices and the provision of information about the specific contributions of each author.

[32] Journal Impact Factor (JIF) by Clarivate (provider for Web of Science)

[33] http://www.eigenfactor.org/

[34] http://www.scimagojr.com/

9. Whether a journal is open-access or subscription-based, remove all reuse limitations on reference lists in research articles and make them available under the Creative Commons Public Domain Dedication[35].

➔ we decidedly encourage publishers to publish all relevant metadata (references, affiliations, license information) via Crossref (see also OpenCitations Initiative)

10. Remove or reduce the constraints on the number of references in research articles, and, where appropriate, mandate the citation of primary literature in favor of reviews in order to give credit to the group(s) who first reported a finding.

**For Organizations That Supply Metrics**

11. Be open and transparent by providing data and methods used to calculate all metrics.

➔ we deliver the complete set of raw data to the MPG clients along with a detailed description of methods

12. Provide the data under a licence that allows unrestricted reuse, and provide computational access to data, where possible.

➔ MPG clients are free to reuse any data provided within the constraints of the underlying licenses (including commercial data providers)

13. Be clear that inappropriate manipulation of metrics will not be tolerated; be explicit about what constitutes inappropriate manipulation and what measures will be taken to combat this.

➔ we invest in the build up of documentation and explanatory material to make it easier to understand metrics and sources of unintended bias

14. Account for the variation in article types (e.g., reviews versus research articles), and in different subject areas when metrics are used, aggregated, or compared.

➔ we apply widley used approaches and invest in further development of appropriate strategies for coping with biases of that kind

**For Researchers**

15. When involved in committees making decisions about funding, hiring, tenure, or promotion, make assessments based on scientific content rather than publication metrics.

➔ see 2.

16. Wherever appropriate, cite primary literature in which observations are first reported rather than reviews in order to give credit where credit is due.

17. Use a range of article metrics and indicators on personal/supporting statements, as evidence of the impact of individual published articles and other research outputs [36].

➔ see 3.

18. Challenge research assessment practices that rely inappropriately on Journal Impact Factors and promote and teach best practice that focuses on the value and influence of specific research outputs.

➔ in our workshops for research coordinators and librarians we explicitly discourage practices that inappropriately rely on JIFs.

[35] http://opencitations.wordpress.com/2013/01/03/open-letter-to-publishers
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