The DESY Research Unit Mat-DMC

Helmholtz Program: From Matter to Materials and Life (MML)

PoF III MML Research Theme: Extreme States of Matter: From Cold Ions to Hot Plasmas

DESY Research Unit: Matter – Dynamics, Mechanisms, and Control (Mat-DMC)

Robin Santra
Center Evaluation DESY, 5 – 9 February 2018

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY

Mat-DMC

Principal Investigators

+ FLASH scientists



Francesca Calegari (DESY & UHH), Henry Chapman (DESY & UHH), Franz Kärtner (DESY & UHH),




Jochen Küpper (DESY & UHH), Tim Laarmann (DESY), Hanns-Peter Liermann (DESY), Nina Rohringer (DESY & UHH),



Ralf Röhlsberger (DESY & UHH), Robin Santra (DESY & UHH), Melanie Schnell (DESY & Universitaet Kiel)

Mat-DMC

What we do

Mat-DMC: Matter—Dynamics, Mechanisms, and Control

- Exploring fundamental aspects of the *dynamics* of matter
- Identifying the underlying *mechanisms*
- Devising microscopic *control* strategies

We provide the conceptual and methodological backbone for all scientific activities employing cutting-edge light sources such as X-ray free-electron lasers.

Research areas

- Short-wavelength nonlinear spectroscopy and quantum optics
- Extreme states of matter
- Molecular reaction pathways
- Attosecond science

PoF-III Research Theme 1

Extreme States of Matter (ESM): From Cold Ions to Hot Plasmas

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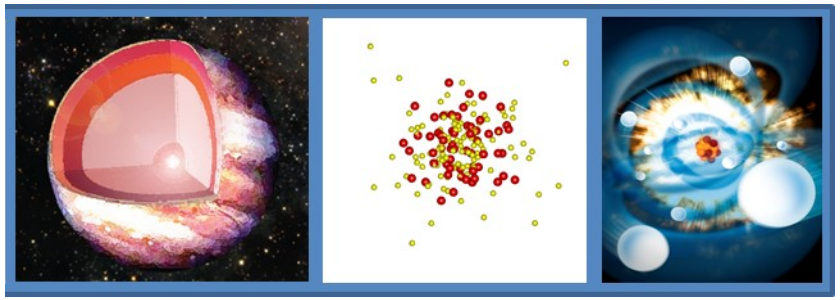
DESY contributes to 4 of the 5 ESM research areas:

- Electromagnetic interactions in matter of high density and/or temperature (ESM.2)
- Molecular imaging and ultrafast dynamics (ESM.3)
- Theory (ESM.4)
- Enabling technologies (ESM.5)



All ESM milestones related to “Mat-DMC” research at DESY have been reached or are on track:

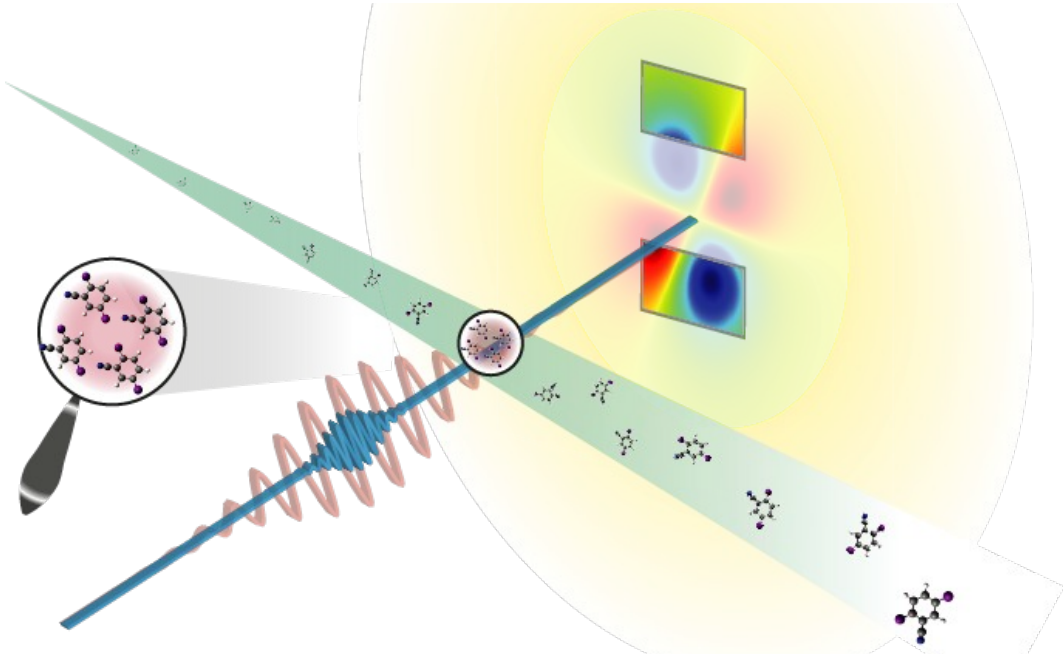
- “First demonstration of novel phasing techniques, making use of modifications of atomic scattering factors by high X-ray intensities, for molecular imaging using X-ray FELs (2016)”
- “Disentangling the stereochemistry of prototypical ring-formation (cycloaddition) reactions (2017)”
- “Availability of first-principles electronic-structure software suite for modeling the behavior of matter in X-ray FEL beams (2017)”
- “High energy and high average power cryogenically cooled solid-state lasers and coherently combined fiber lasers for strong field experiments at high repetition rate (2017)”
- “Compact laser-driven X-ray sources for seeding of XFELs and attosecond science and spectroscopy at FELs and ion storage rings (2018)”

Achievements

Mat-DMC research area “Molecular reaction pathways”

We play an internationally leading role in state-of-the-art molecular quantum-state-resolved sample preparation and control.

- We have demonstrated atomic-resolution coherent X-ray diffractive imaging of isolated, controlled, strongly aligned gas-phase molecules.



- Chang, Y.-P. et al., Specific Chemical Reactivities of Spatially Separated 3-Aminophenol Conformers with Cold Ca^+ Ions. *Science* **342**, 98–101 (2013).
- Küpper, J. et al., X-Ray Diffraction from Isolated and Strongly Aligned Gas-Phase Molecules with a Free-Electron Laser. *Physical Review Letters* **112**, 083002 (2014).

Contribution to ESM.3.

Achievements

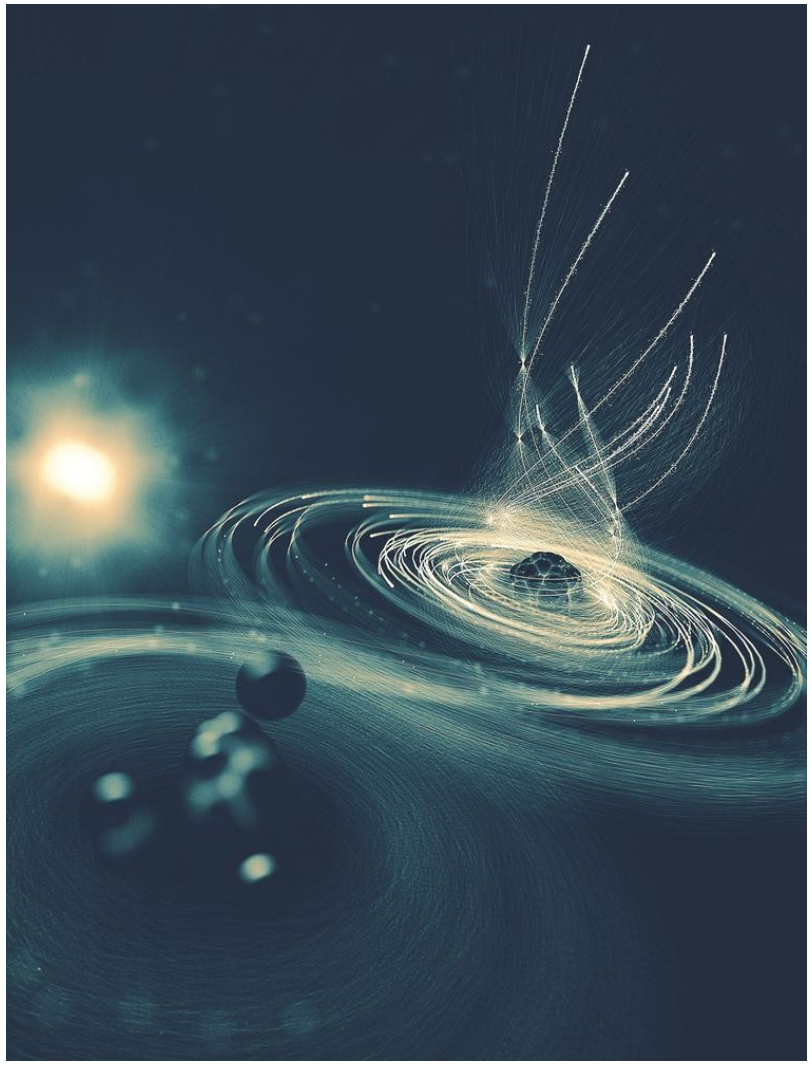
Mat-DMC research area “Extreme states of matter”

We hold a worldwide accepted leadership in developing and utilizing tools for quantitatively simulating the dynamics of matter driven by high-intensity short-wavelength radiation.

- The unique capabilities of our simulation tools have made possible our discovery of a new molecular ionization enhancement mechanism at extremely high X-ray intensity.

- Murphy, B. F. et al., Femtosecond X-ray-induced explosion of C_{60} at extreme intensity.
  Nature Communications **5**, 4281 (2014).
- Rudenko, A. et al., Femtosecond response of polyatomic molecules to ultra-intense hard X-rays.
  Nature **546**, 129–132 (2017).

Contribution to ESM.4.



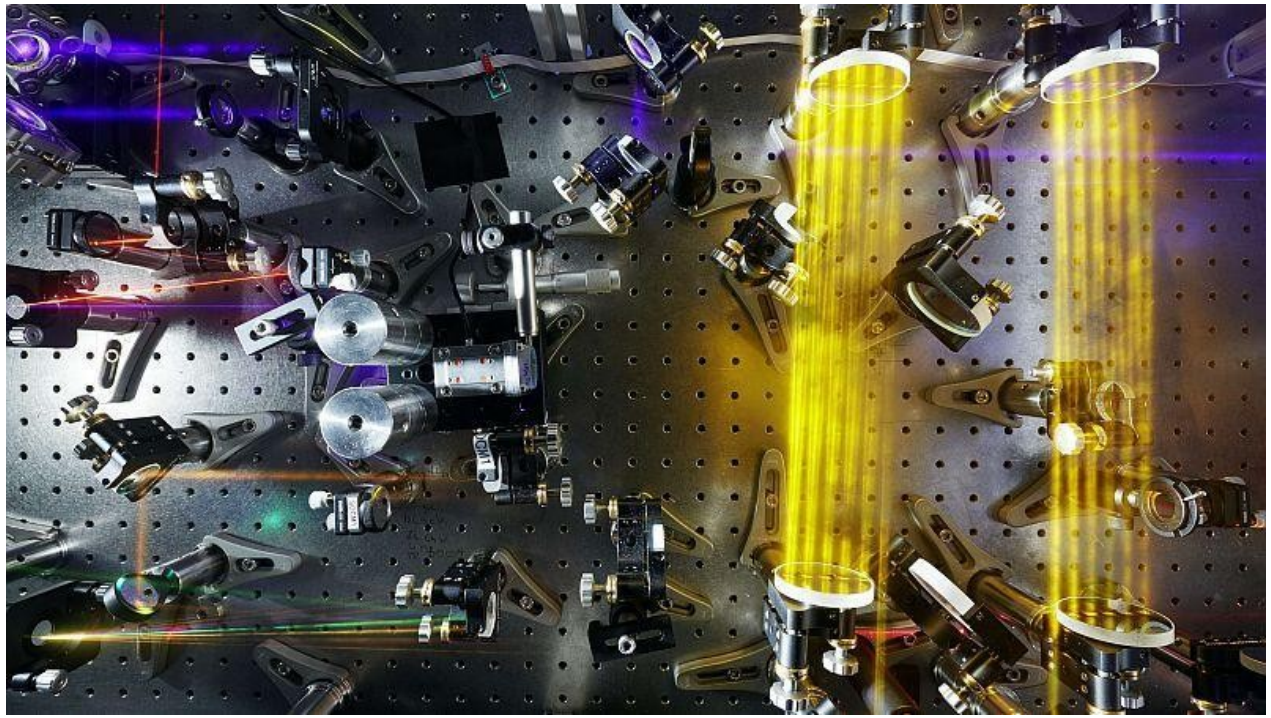
Achievements

Mat-DMC research area “Attosecond science”

As an internationally recognized leader in ultrafast optical technology, we have taken important steps towards unifying attosecond science and X-ray science.

- Our development of multi-octave spanning subcycle optical waveform synthesizers paves the way for advanced control of electrons in attosecond science.

- Krogen, P. et al., Generation and multi-octave shaping of mid-infrared intense single-cycle pulses. *Nature Photonics* **11**, 222–226 (2017).
- Usenko, S. et al., Attosecond Interferometry with Self-Amplified Spontaneous Emission of a free-electron laser. *Nature Communications* **8**, 15626 (2017).



Contribution to ESM.5.

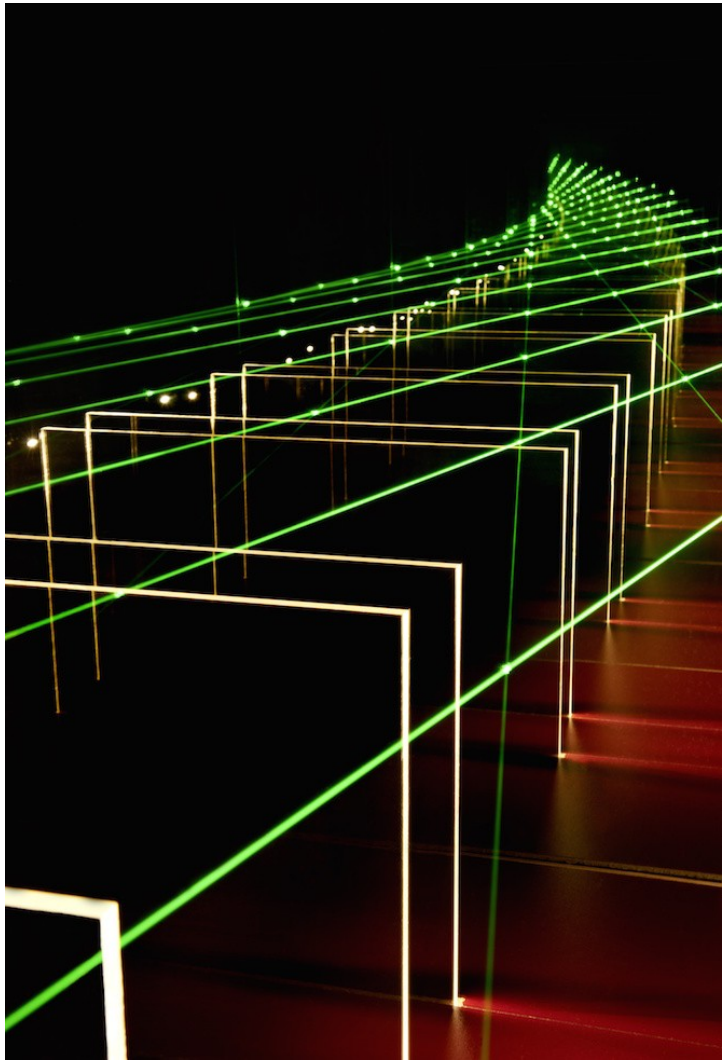
Achievements

Mat-DMC research area “Short-wavelength nonlinear spectroscopy and quantum optics”

Employing X-ray standing waves and Mössbauer nuclei, we are internationally recognized as having established the new field of X-ray nuclear quantum optics.

- Our demonstration of strong coupling between X-rays and nuclei has moved quantum-optical concepts forward into an entirely new regime for fundamental science.

- Haber, J. et al., Collective strong coupling of X-rays and nuclei in a nuclear optical lattice.
  Nature Photonics **10**, 445–449 (2016).
- Haber, J. et al., Rabi oscillations of X-ray radiation between two nuclear ensembles.
  Nature Photonics **11**, 720–725 (2017).



Contribution to PoF III MML RT4
(Nanoscience and materials for information technologies).

Important development within PoF III

New DESY PIs in MML RT1

Francesca Calegari
DESY lead scientist; full professor of physics at Universitaet Hamburg

Nina Rohringer
DESY lead scientist; full professor of physics at Universitaet Hamburg

Melanie Schnell
DESY lead scientist; full professor of physical chemistry at Universitaet Kiel

Talents and Career Development

Ph.D. prizes and postdoctoral fellowships

- Anne-Laure Calendron (Helmholtz postdoctoral fellowship); Johann Haber (Helmholtz Ph.D. Prize); Antonia Karamatskou (Louise Johnson postdoctoral fellowship); Zheng Li (Peter Paul Ewald postdoctoral fellowship); Jolijn Onlvee (Alexander von Humboldt fellowship); Stefan Pabst (Helmholtz Ph.D. Prize); Andrea Trabattoni (Alexander von Humboldt fellowship); Lu Wu (Alexander von Humboldt fellowship)

Emerging Leaders (Journal of Physics B)

- Giovanni Cirmi; Sang-Kil Son

Academic positions

- Yuan-Pin Chang (assistant professor at National Sun Yat-Sen University, Taiwan); Gopal Dixit (assistant professor in the Department of Physics at IIT Mumbai, India); Daniel Rolles (assistant professor in the Department of Physics at Kansas State University, USA); Oriol Vendrell (associate professor in the Department of Physics at Aarhus University); plus nine others who obtained faculty positions at institutions ranging from Cornell University, University of Colorado at Boulder, Boston University, to Beihang University in Beijing, China.

Other recognitions and awards

- Francesca Calegari (ERC Starting Grant); Jochen Küpper (ERC Consolidator Grant; Fellow of the Royal Society of Chemistry); Ralf Röhlsberger (Björn Wiik Prize); Robin Santra (Fellow of the American Physical Society); Melanie Schnell (ERC Starting Grant)

Proposed PoF-IV Research Topic 1

Matter—Dynamics, Mechanisms, and Control (Mat-DMC)

Proposed research themes

- Nonperturbative fields and quantum optics
- Matter under extreme conditions
- Molecular reaction pathways
- Electronic structure and driven states of matter
- Attosecond science
- Science-driven instrumentation and methodology

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Particular goals for DESY

- Our research will continue to be partly curiosity-driven, partly methodology-driven, and partly need-driven.
- It remains our declared mission to contribute to developing the science opportunities at PETRA III/IV, at FLASH, and at the European XFEL.
- We will continue to play a prominent role in shaping the research activities of the Hamburg Center for Ultrafast Imaging, within the framework of the German Excellence Initiative.
- We plan on expanding our efforts in investigating geophysically and astrophysically relevant, extreme states of matter.
- We will actively support the development of attosecond science capabilities at FLASH (FLASH 2020).