

# Science at European XFEL

Thomas Feurer





Photo: Deutsche Photothek / Franz Stoedtner

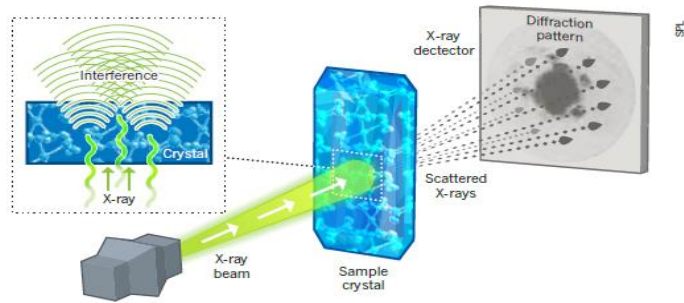
$$d = \frac{\lambda}{2n \sin \alpha}$$

# ATOMIC SECRETS

## 100 YEARS OF CRYSTALLOGRAPHY

BY NICOLA JONES

In 1914, German scientist Max von Laue won the Nobel Prize in Physics for discovering how crystals can diffract X-rays: a phenomenon that led to the science of X-ray crystallography. Since then, researchers have used diffraction to work out the crystalline structures of increasingly complex molecules, from simple minerals to high-tech materials such as graphene and biological structures, including viruses. With improvements in technology, the pace of discovery has accelerated: tens of thousands of new structures are now imaged every year. The resolution of crystallographic images of proteins passed a critical threshold for discriminating single atoms in the 1990s, and newer X-ray sources promise images of challenging proteins that are hard or impossible to grow into large crystals.



### BIRTH OF AN IDEA

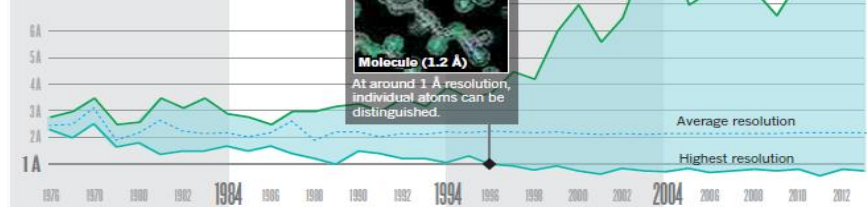
Von Laue hit on the idea that when X-rays passed through a crystal, they would scatter off the atoms in the sample and then interfere with each other like waves passing through a breach in a shore wall. In some places, the waves would add to each other; in others, cancel each other out. The resulting diffraction pattern could be used to back-calculate the location of the atoms that scattered the original X-rays. Von Laue and his colleagues proved his theory in 1912 with a sample of copper sulphate.

- 1913** **DIAMOND**  
Diffraction image allowed researchers to confirm the tetrahedral structure of carbon atoms in this famous crystal.
- 1923** **HEXAMETHYLENE-TETRAMINE**  
The first organic molecule to be imaged, chosen because of its simple cubic symmetry. It proved that molecules, not just atoms, can make up the repeating elements of a crystal.
- 1925** **QUARTZ**  
The determination of the structure of silicate minerals was fundamental to the field of mineralogy.
- 1929** **HEXAMETHYLENE-TETRAMINE** (continued)
- 1952** **DNA**  
Rosalind Franklin's X-ray image of DNA, known as photo 51, helped James Watson and Francis Crick to create their famous model of the double helix. An atomic-resolution image of the structure proposed in 1953 was not taken until 1980.
- 1958** **MYOGLOBIN**  
The irregular folds seen in the structure of the first imaged protein were a huge surprise.
- 1965** **LYSOZYME**  
The first enzyme to be imaged, sourced from hen egg whites.
- 1970** **SYNCHROTRON**  
A study of insect muscle at the German Electron Synchrotron (DESY) in Hamburg was the first to use X-rays generated by a synchrotron. The use of these machines caused a boom in crystallography studies.

IMAGES: BERNHARD RUPP/GARLAND SCIENCE/TAYLOR & FRANCIS; GRAPH: H. M. BERMAN/PROTEIN SCI., 21, 1987-1, 596 (2012), WITH UPDATES FROM WORLDWIDE PROTEIN DATA BANK

### GETTING CLEARER

Better techniques for both imaging and interpreting data have allowed researchers see finer details in some structures and tackle ever more complicated molecules.



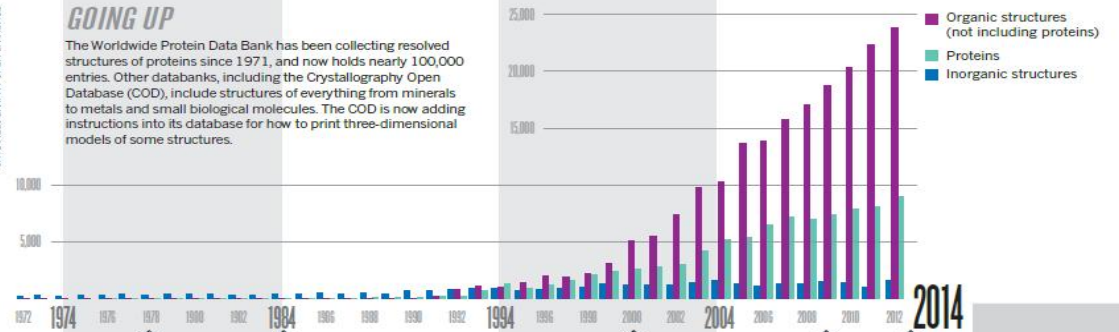
Resolution suffers in images of some complex structures, often because of variations or motion within a crystal.

The average resolution of proteins imaged through crystallography has not changed much; advances in resolution are balanced by attempts to image more complex structures.

SOURCE: WORLDWIDE PROTEIN DATA BANK/CRYSTALLOGRAPHY OPEN DATABASE

### GOING UP

The Worldwide Protein Data Bank has been collecting resolved structures of proteins since 1971, and now holds nearly 100,000 entries. Other databanks, including the Crystallography Open Database (COD), include structures of everything from minerals to metals and small biological molecules. The COD is now adding instructions into its database for how to print three-dimensional models of some structures.



- 1978** **TOMATO BUSHY STUNT VIRUS**  
First atomic-scale image of a complete virus: in this case, a plant virus. It revealed structural rules that were found to hold true in human pathogens a few years later.
- 1984** **QUASICRYSTALS**  
The first crystals were identified with atomic arrangements that do not repeat exactly, defying general wisdom about crystals.
- 2000** **RIBOSOME**  
The molecular machine that assembles proteins from instructions encoded in DNA.
- 2009** **X-RAY FREE-ELECTRON LASER**  
The Linac Coherent Light Source at the SLAC National Accelerator Laboratory in Menlo Park, California, went into operation, opening up a new world of imaging possibilities (see page 604).
- 2013** **HIV TRIMER**  
An X-ray crystallographic image of the hook that HIV uses to bind to human cells helped to resolve a debate about what this important protein looks like.

### THE FUTURE

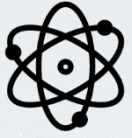
The 'most wanted' list of proteins that remain to be imaged includes the massive spliceosome, which helps to organize, edit messenger RNA, and the even larger nuclear-pore complex, which serves as a nucleus's gatekeeper.

These structures can contain hundreds of proteins, making them hard to crystallize or keep still for an image.

One strategy is to crystallize bits of these structures and piece them together like a jigsaw; the use of X-ray free-electron lasers should also help.

**CRYSTALLOGRAPHY AT 100**  
A Nature special issue  
[nature.com/crystallography](http://nature.com/crystallography)

# What does European XFEL do?



## Stars

Extreme heat and pressure;  
pathways toward fusion energy



## Artificial Photosynthesis

Learning from plants  
to turn sunlight into fuels



## Planets and exoplanets

Interiors, magnetic fields,  
and diamond rain

## Biology

Proteins and enzymes in  
action; biological magnetic  
sensing



## Catalysis

Catalysts observed in action  
for cleaner reactions



## Humans

Structures and functions  
of human proteins and enzymes



At a glance

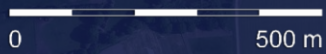
Schleswig-Holstein

Hamburg

Schenefeld

Osdorfer Born

DESY-Bahrenfeld



Schleswig-Holstein

Hamburg

Schenefeld

Osdorfer Born

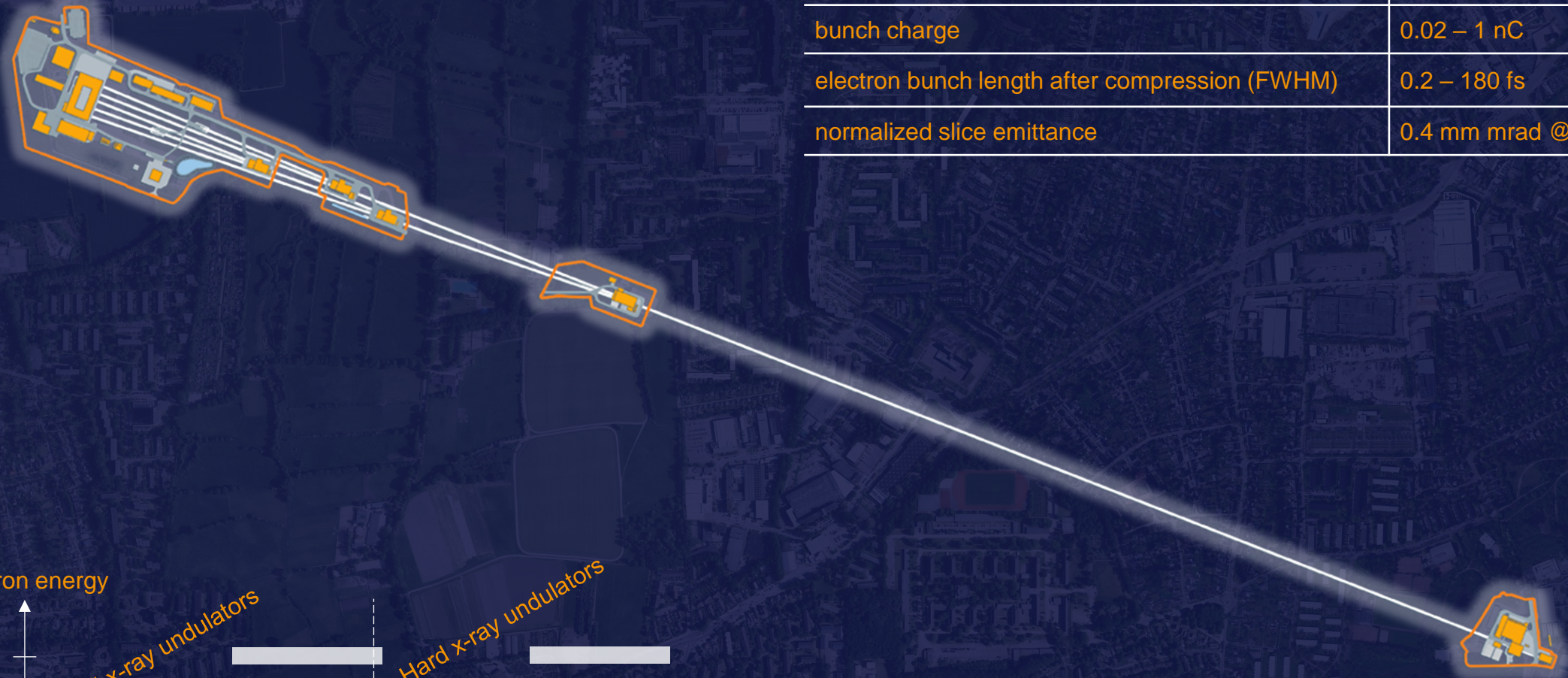
DESY-Bahrenfeld



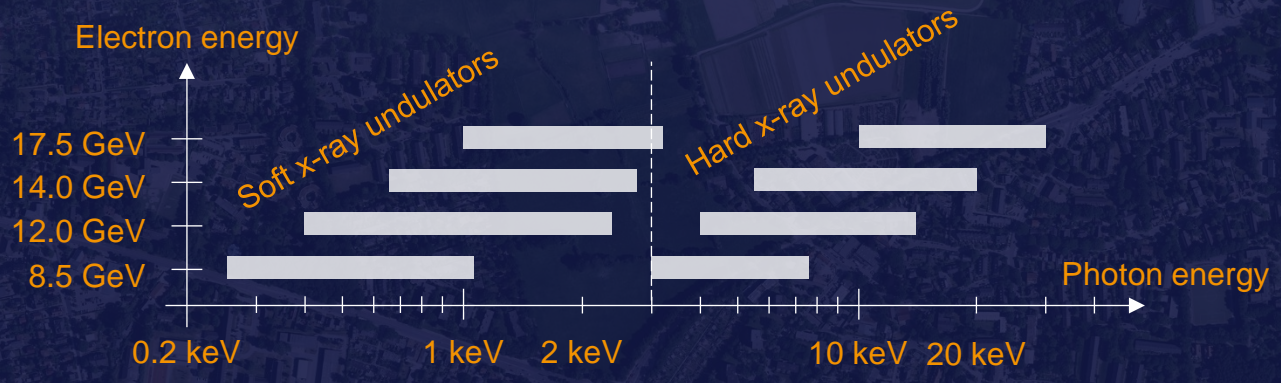
0

500 m





electron beam energy	6 - 17.5 GeV
# of bunches/second	27,000
bunch charge	0.02 – 1 nC
electron bunch length after compression (FWHM)	0.2 – 180 fs
normalized slice emittance	0.4 mm mrad @ 0.25 nC

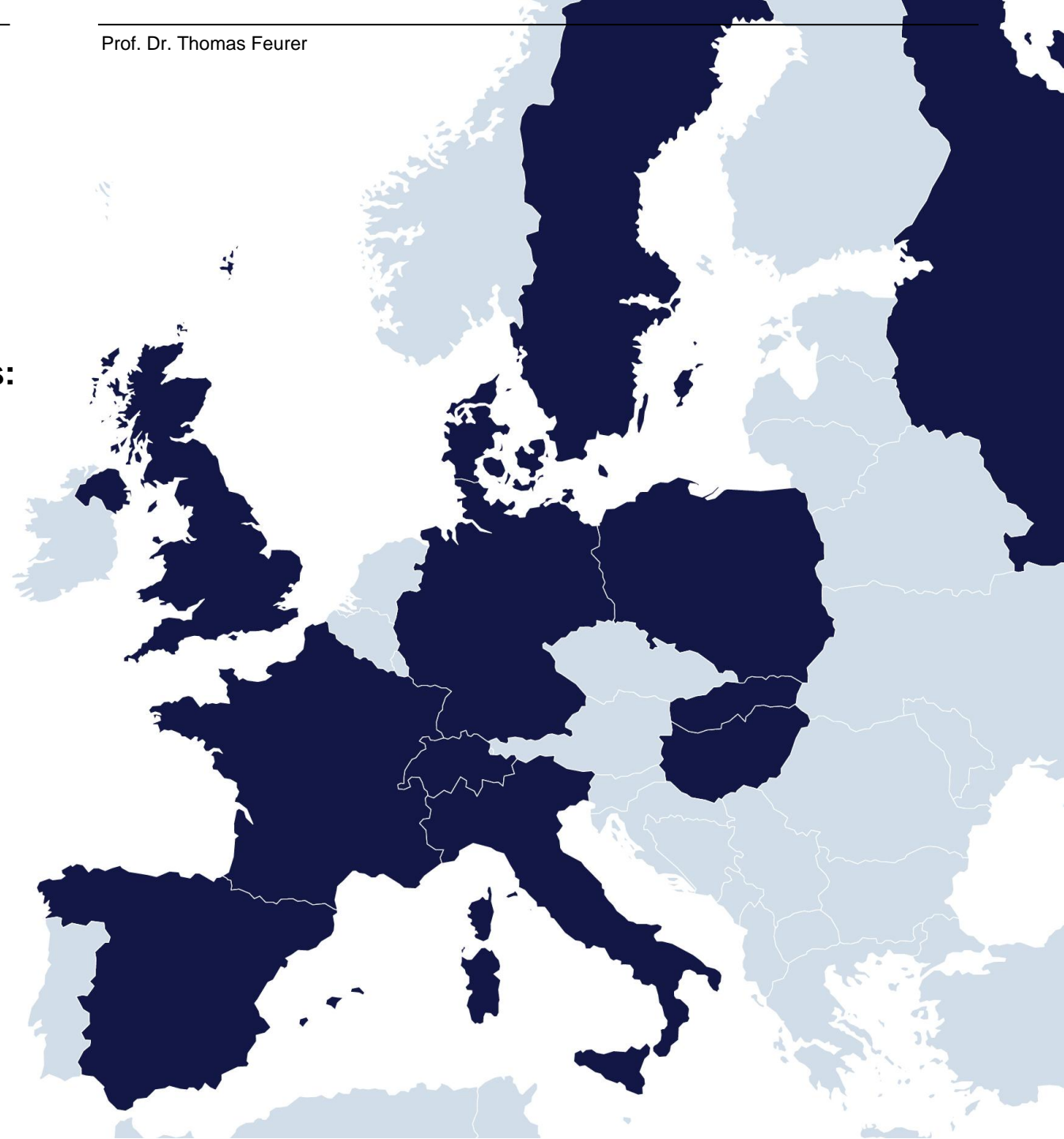


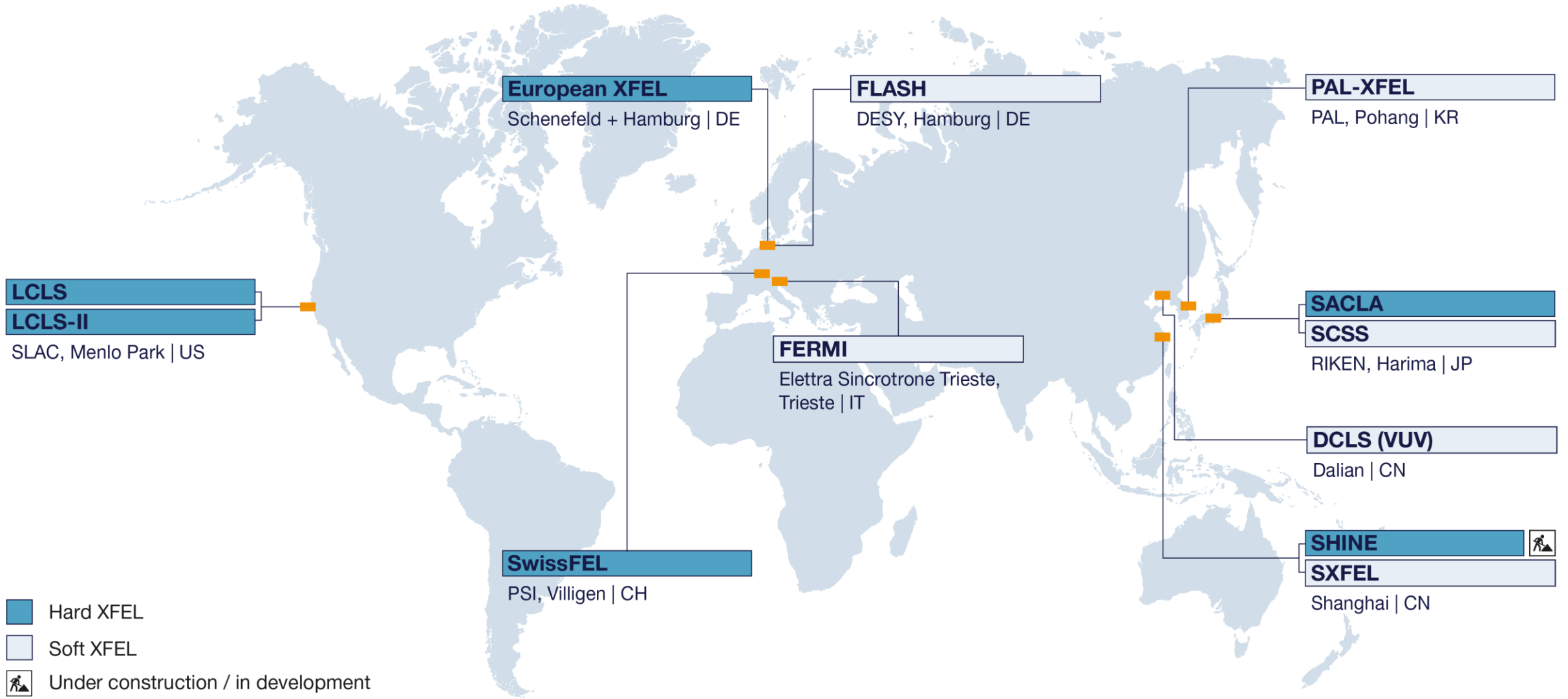




# European XFEL – a research facility of superlatives

- **Non-profit company with 12 shareholding countries:**
- Germany (Bund, Hamburg and Schleswig-Holstein) covers 57% shares, Russia 26%
- Other shareholders at 1–3% each
  
- **Construction costs:** 1.54 billion € (as of 2018)
- **Annual budget:** about 150 million €



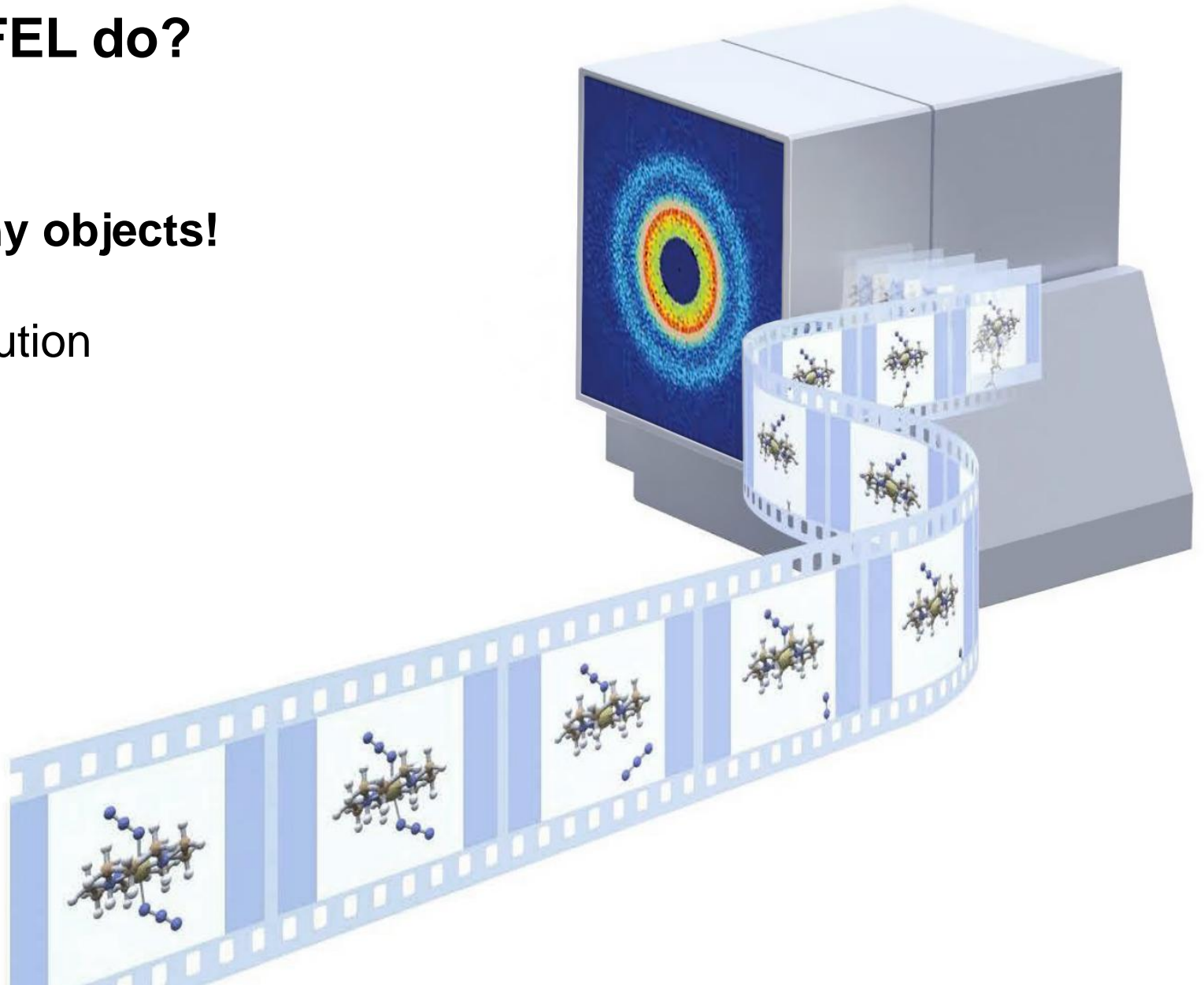


# What does European XFEL do?

**A big facility for studying tiny objects!**

X-ray light: reach atomic resolution

Ultrashort flashes:  
film (bio-)chemical reactions



# Scientific instruments



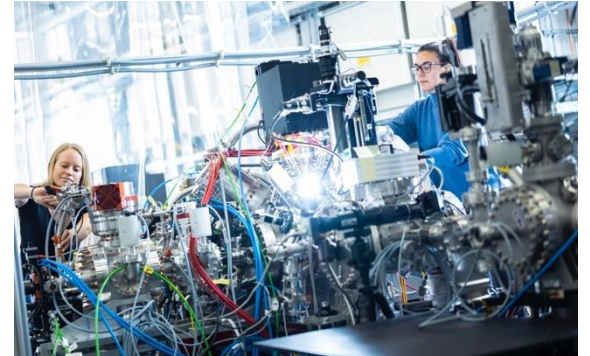
**FXE** (film very fast reactions)



**SPB/SFX** (focus on biomolecules)



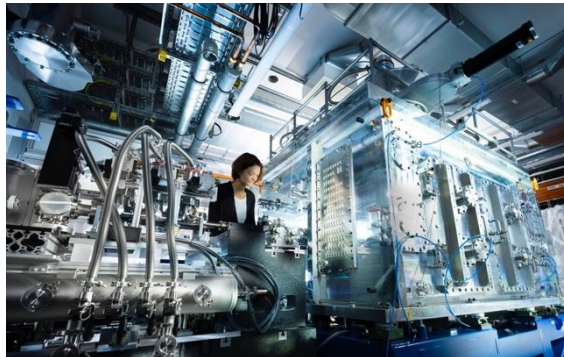
**SCS** (look at processes of materials and liquids)



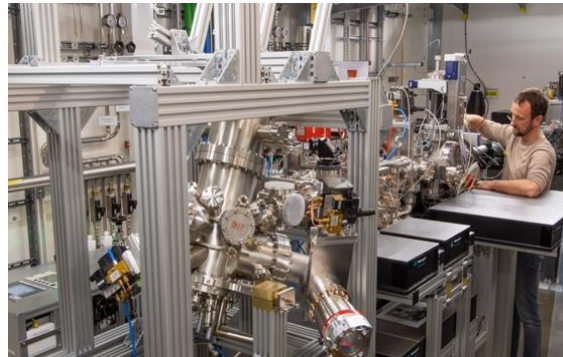
**SQS** (basis research of reactions of molecules and small clusters)



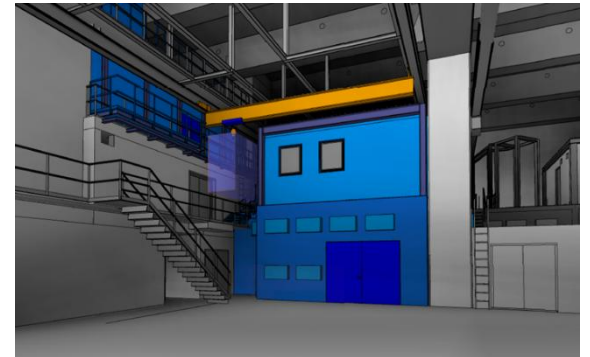
**MID** (diverse applications in materials research)



**HED** (matter under extreme conditions)

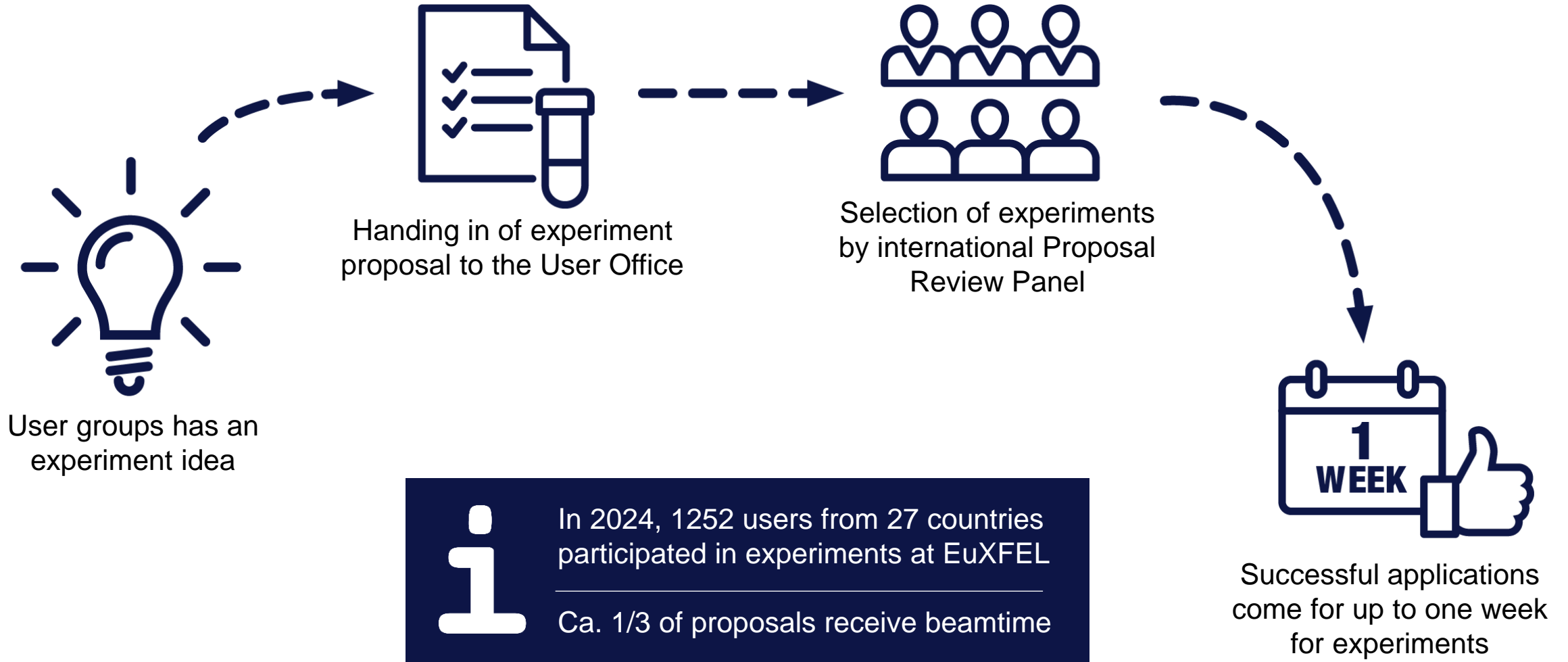


**SXP** (look at electrons and chemical reactions)



**HXS** (material research)  
**under construction**

## A user facility





**7**

instruments, plus 1 under construction



**27000**

electron bunches per second



**580**

staff members incl. guests



**>30**

PB of raw data collected per year



**1252**

individual annual users



**96**

user experiments per year



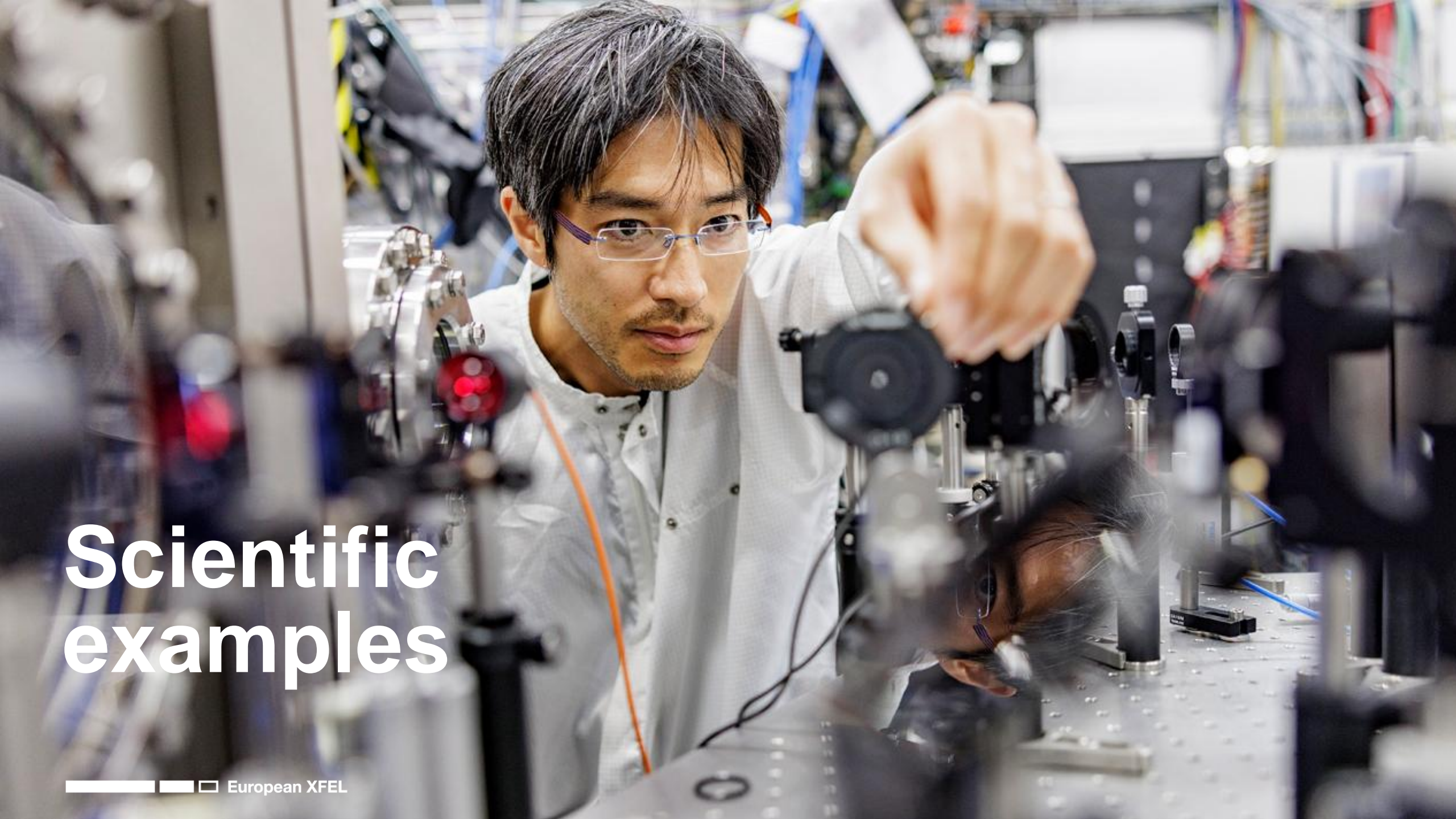
**>1500**

total publications

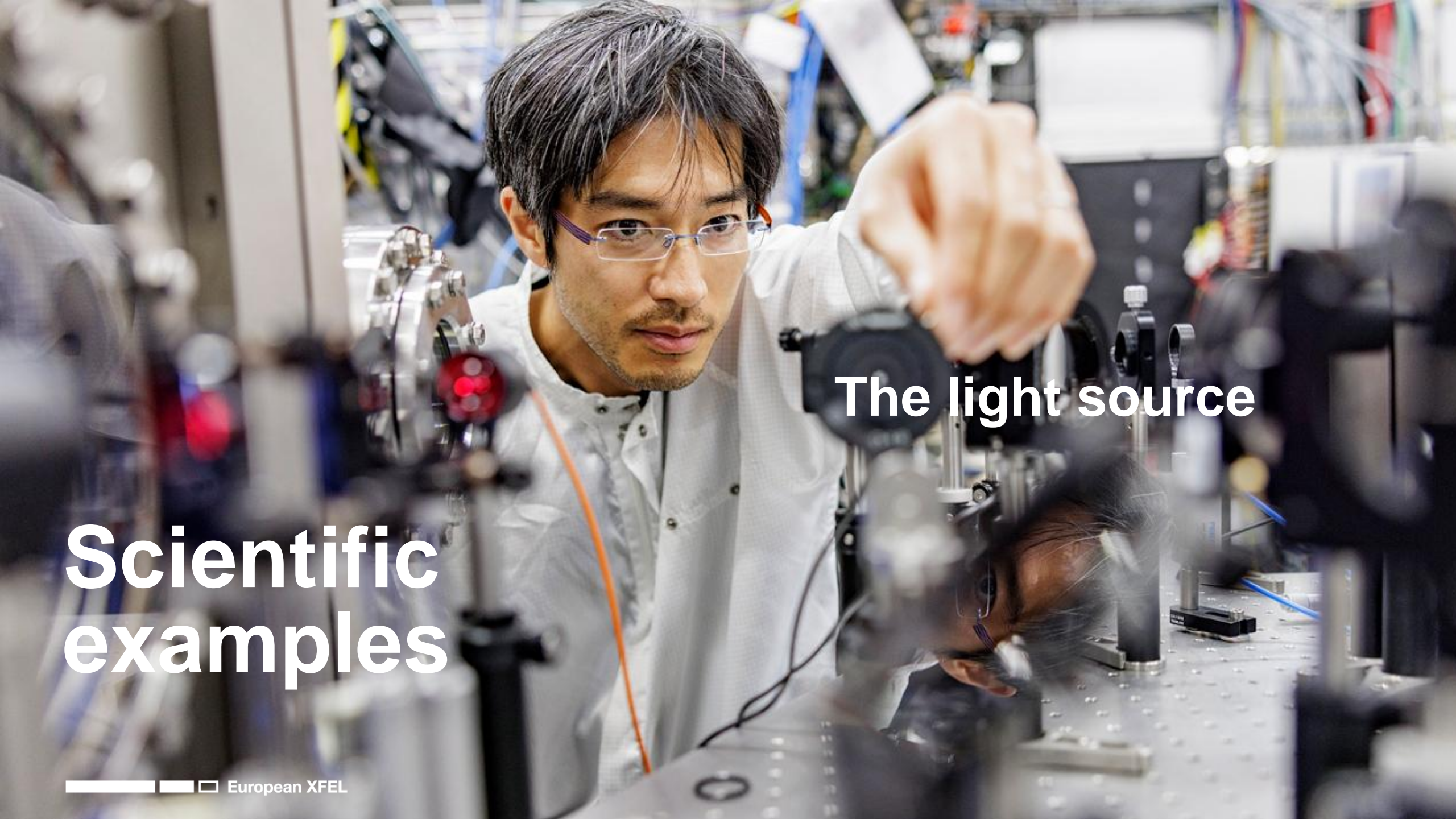


**28000**

cups of coffee served per year in the campus restaurant BeamStop



# Scientific examples



The light source

Scientific  
examples

# Journal of

VOLUME 73, NUMBER 1

PHYSICAL REVIEW LETTERS

4 JULY 1994

## Spectrum, Temporal Structure, and Fluctuations in a High-Gain Free-Electron Laser Starting from Noise

R. Bonifacio,<sup>1,2</sup> L. De Salvo,<sup>1</sup> P. Pierini,<sup>2</sup> N. Piovella,<sup>1</sup> and C. Pellegrini<sup>3</sup>

<sup>1</sup>*Dipartimento di Fisica dell'Università di Milano, Via Celoria 16, 20133 Milano, Italy*

<sup>2</sup>*Istituto Nazionale di Fisica Nucleare-Sezione di Milano, Via Celoria 16, 20133 Milano, Italy*

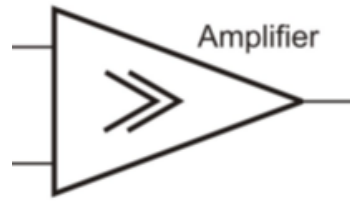
<sup>3</sup>*Department of Physics, University of California Los Angeles, 405 Hilgard Avenue, Los Angeles, California 90024*

(Received 14 July 1993)

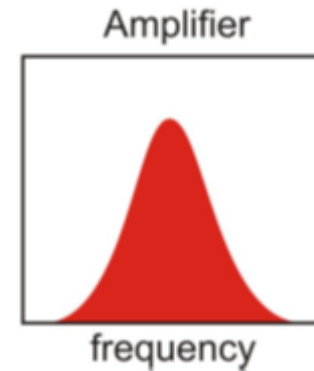
We study the time structure, the frequency composition, and the shot to shot fluctuations of the radiation emitted by a free-electron laser starting from shot noise in the electron beam longitudinal distribution, taking into account slippage and finite bunch length effects. We find a very different behavior when the bunch length,  $\ell_b$ , is much longer than the cooperation length,  $\ell_c$ , or of the order of a few  $\ell_c$ . The field evolution is dominated by slippage effects in both cases, and shows the presence of superradiant spikes.

It is concluded that several applications of the radiation appear possible. A scheme for obtaining millimeter-waves of considerable power is outlined. The upper limit of the power in a band extending down to a wavelength of 1 millimeter is calculated to be of the order of several kilowatts for a beam of one ampere and an energy of 1.5 megavolt. The use of the radiation for speed monitoring of beams with energies up to 1000 megavolt is discussed.

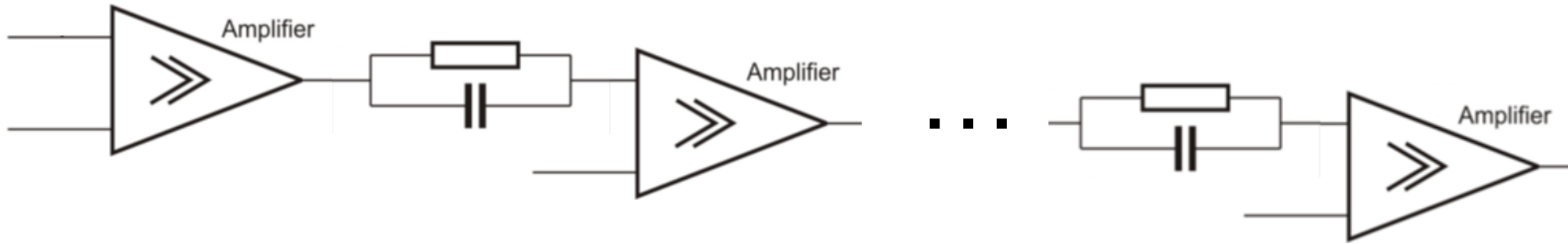
# A free-electron laser is a classical amplifier



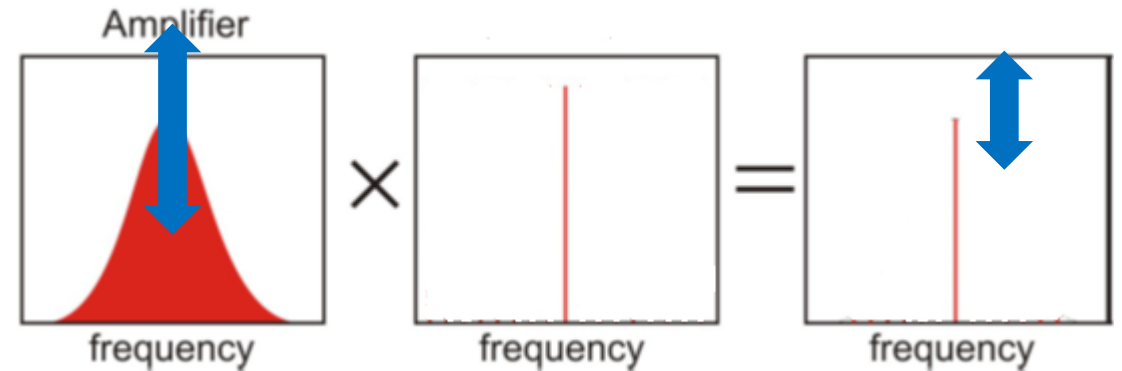
An amplifier with no input amplifies shot noise within its gain curve. The output is a noisy, incoherent spectrum (**SASE**).



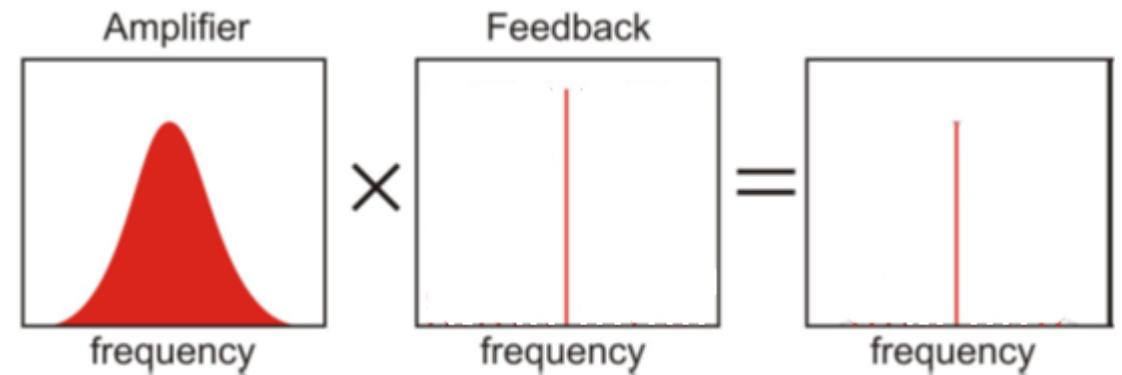
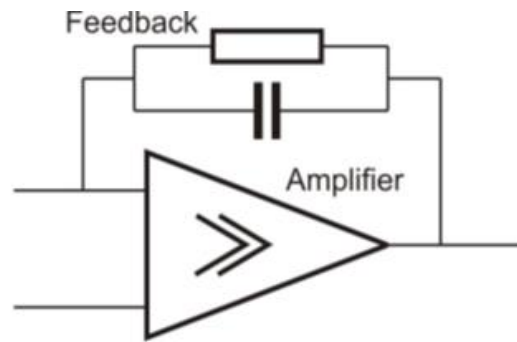
# Increasing spectral brightness



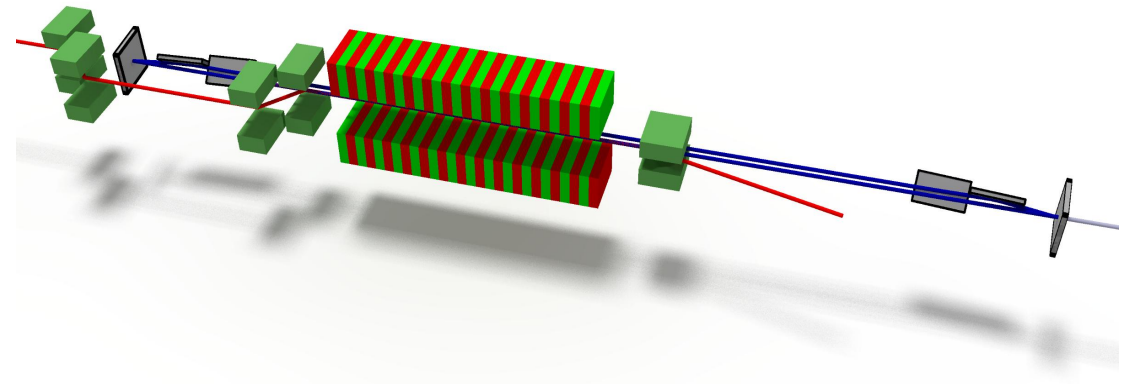
The first amplifier produces amplified noise (SASE) within its gain curve. The output is filtered and amplified further. Saturation reduces amplitude fluctuations (**Self Seeding**).



# From an amplifier to an oscillator

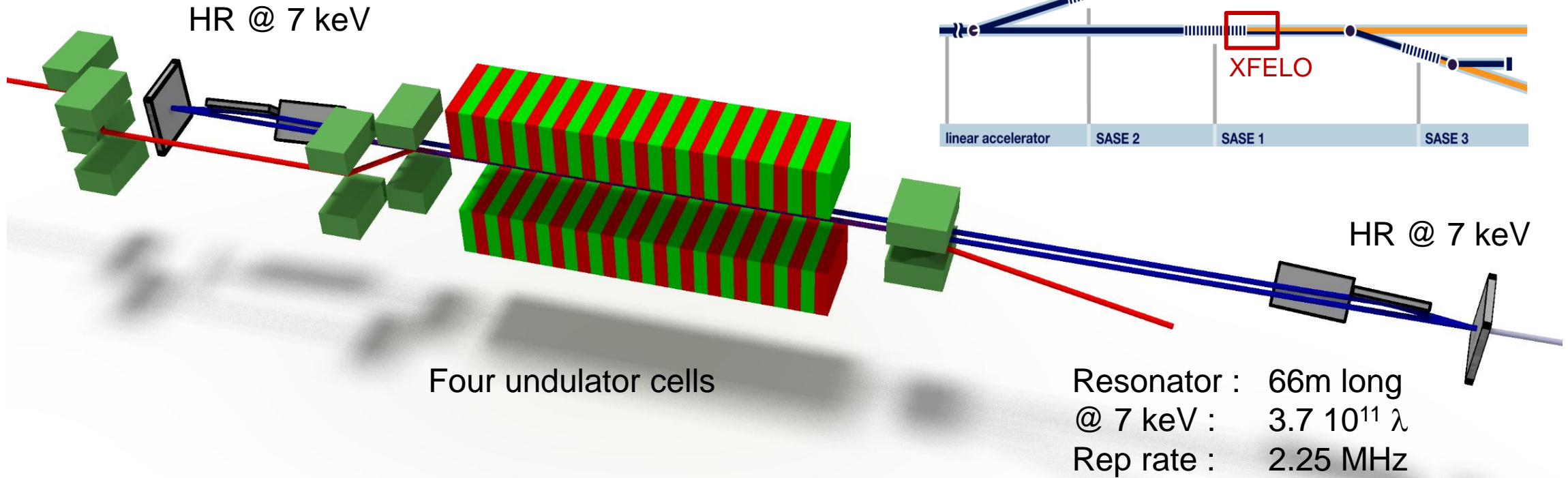


When part of the output is filtered and fed back to the input, a well defined (by feedback) coherent output is generated (**Laser**).

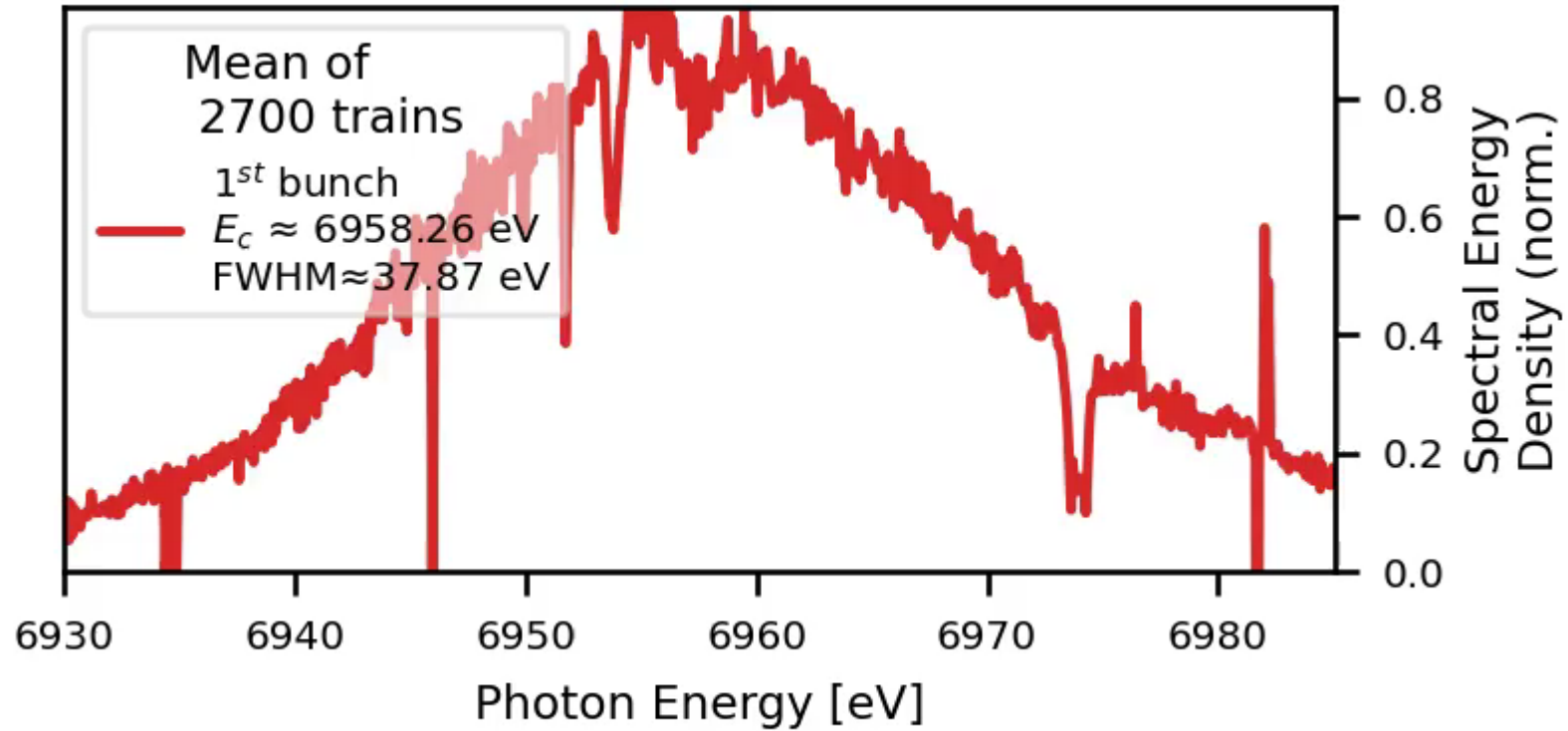


# XFELO demonstrator project

**XFELO** = **X**-ray **F**ree **E**lectron **L**aser **O**scillator



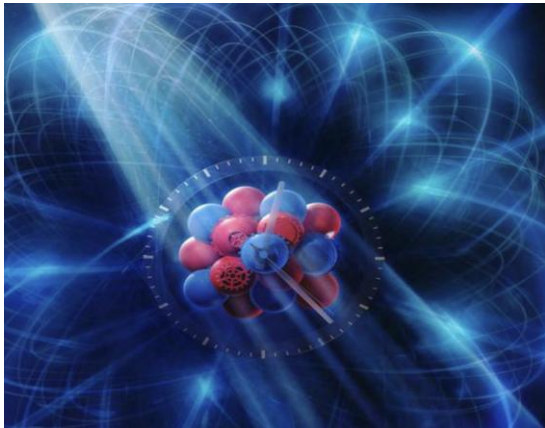
# The first ever hard X-ray laser oscillator



# A fantastic team effort and a fantastic piece of mechanical engineering

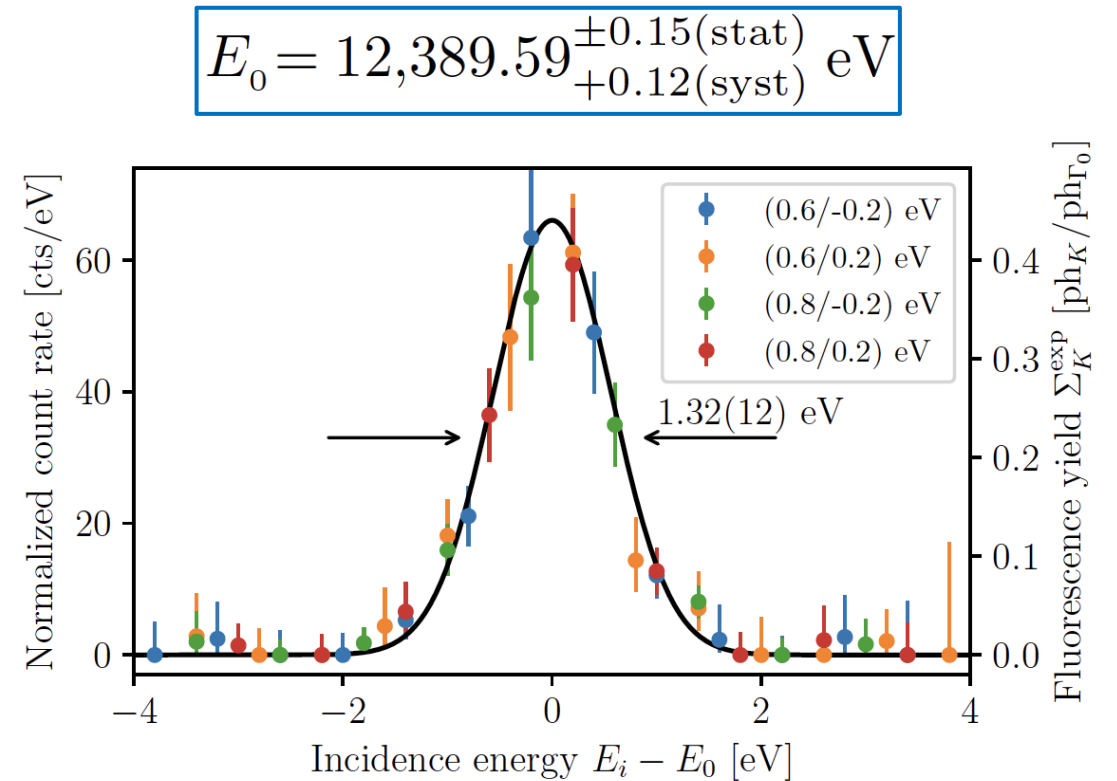


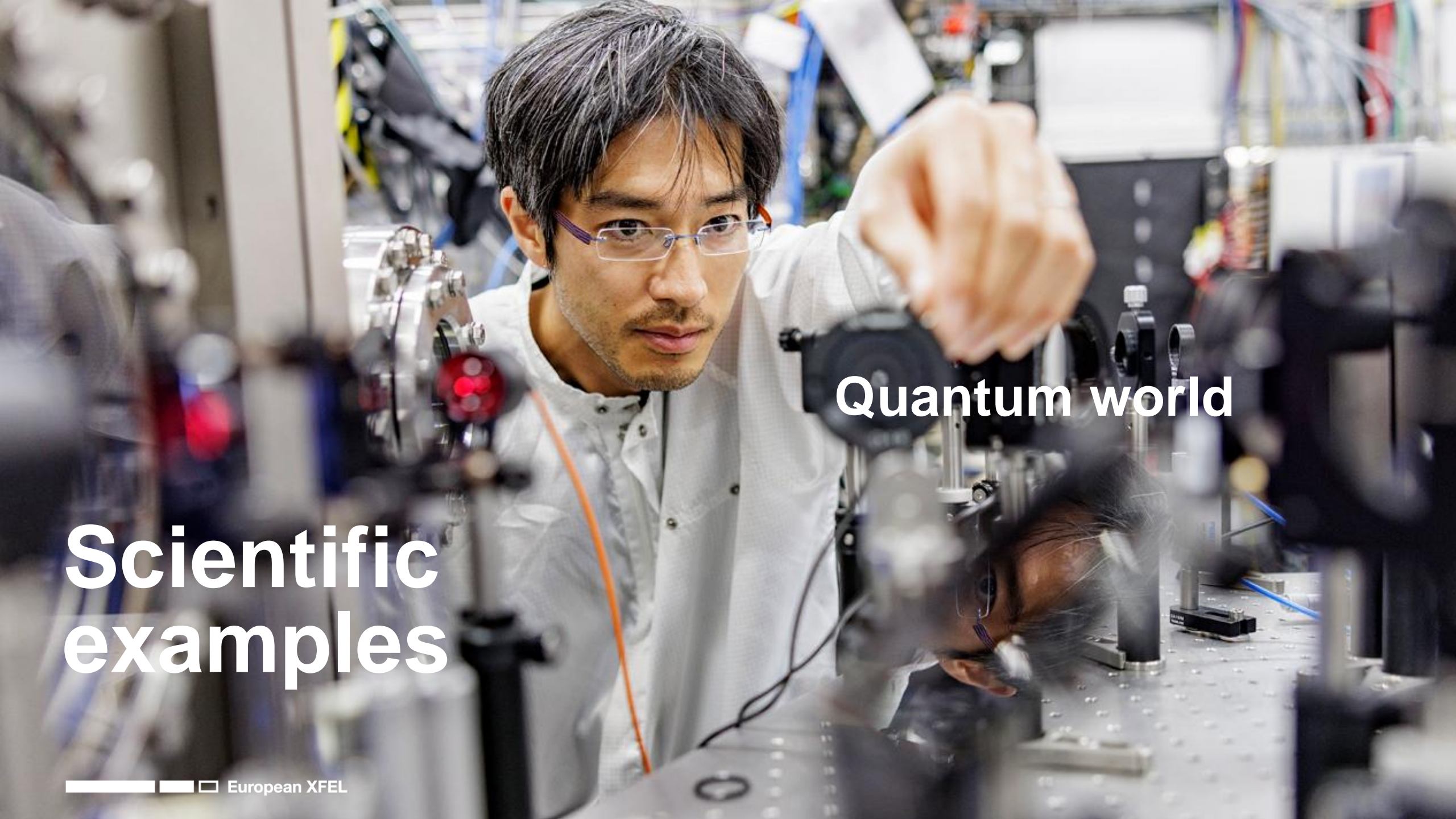
# Resonant excitation of the nuclear clock isomer $^{45}\text{Sc}$



■ Nuclear clocks are the world's most accurate timekeepers, required for functionalities such as precise positioning using satellite navigation

- Resonant oscillators with stable frequencies
- Nuclear oscillators surpass their atomic counterparts by higher quality factors and resilience against external perturbations
- The 12.4 keV nuclear transition in  $^{45}\text{Sc}$
- **Ultranarrow transition linewidth: 1.4 feV**





Quantum world

Scientific  
examples

Article | [Open access](#) | Published: 21 February 2022

# X-ray multiphoton-induced Coulomb explosion images complex single molecules

[Rebecca Boll](#) , [Julia M. Schäfer](#), [Benoît Richard](#), [Kilian Fehre](#), [Gregor Kastirke](#), [Zoltan Jurek](#), [Markus S. Schöffler](#), [Malik M. Abdullah](#), [Nils Anders](#), [Thomas M. Baumann](#), [Sebastian Eckart](#), [Benjamin Erk](#), [Alberto De Fanis](#), [Reinhard Dörner](#), [Sven Grundmann](#), [Patrik Grychtol](#), [Alexander Hartung](#), [Max Hofmann](#), [Markus Ilchen](#), [Ludger Inhester](#), [Christian Janke](#), [Rui Jin](#), [Max Kircher](#), [Katharina Kubicek](#), [Maksim Kunitski](#), [Xiang Li](#), [Tommaso Mazza](#), [Severin Meister](#), [Niklas Melzer](#), [Jacobo Montano](#), [Valerija Music](#), [Giammarco Nalin](#), [Yevheniy Ovcharenko](#), [Christopher Passow](#), [Andreas Pier](#), [Nils Rennhack](#), [Jonas Rist](#), [Daniel E. Rivas](#), [Daniel Rolles](#), [Ilme Schlichting](#), [Lothar Ph. H. Schmidt](#), [Philipp Schmidt](#), [Juliane Siebert](#), [Nico Strenger](#), [Daniel Trabert](#), [Florian Trinter](#), [Isabel Vela-Perez](#), [Rene Wagner](#), [Peter Walter](#), [Miriam Weller](#), [Pawel Ziolkowski](#), [Sang-Kil Son](#), [Artem Rudenko](#), [Michael Meyer](#), [Robin Santra](#)  & [Till Jahnke](#)  — Show fewer authors

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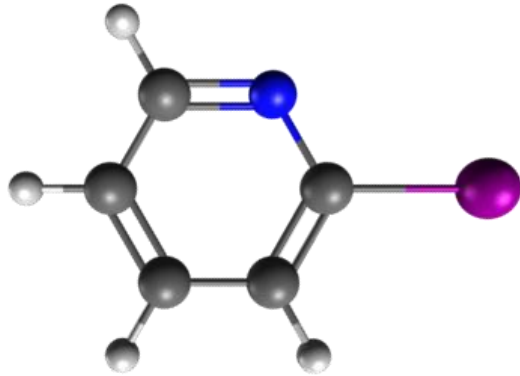


Rebecca Boll

## Imaging collective quantum fluctuations of the structure of a complex molecule

Benoît Richard<sup>1,2,3</sup>, Rebecca Boll<sup>4\*</sup>, Sourav Banerjee<sup>1</sup>, Julia M. Schäfer<sup>1,5</sup>, Zoltan Jurek<sup>1</sup>, Gregor Kastirke<sup>6,7</sup>, Kilian Fehre<sup>6</sup>, Markus S. Schöffler<sup>6</sup>, Nils Anders<sup>6</sup>, Thomas M. Baumann<sup>4</sup>, Sebastian Eckart<sup>6</sup>, Benjamin Erk<sup>8</sup>, Alberto De Fanis<sup>4</sup>, Reinhard Dörner<sup>6,7</sup>, Sven Grundmann<sup>6</sup>, Patrik Grychtol<sup>4</sup>, Max Hofmann<sup>6</sup>, Markus Ilchen<sup>1,2,4</sup>, Max Kircher<sup>6</sup>, Katharina Kubicek<sup>2,3,4</sup>, Maksim Kunitski<sup>6</sup>, Xiang Li<sup>9,10</sup>, Tommaso Mazza<sup>4</sup>, Severin Meister<sup>11</sup>, Niklas Melzer<sup>6</sup>, Jacobo Montano<sup>4</sup>, Valerija Music<sup>4,12</sup>, Yevheniy Ovcharenko<sup>4</sup>, Christopher Passow<sup>8</sup>, Andreas Pier<sup>6</sup>, Nils Rennhack<sup>4</sup>, Jonas Rist<sup>6</sup>, Daniel E. Rivas<sup>4</sup>, Daniel Rolles<sup>9</sup>, Ilme Schlichting<sup>13</sup>, Lothar Ph. H. Schmidt<sup>6</sup>, Philipp Schmidt<sup>4,12</sup>, Daniel Trabert<sup>6</sup>, Florian Trinter<sup>6,14</sup>, Rene Wagner<sup>4</sup>, Peter Walter<sup>10</sup>, Pawel Ziolkowski<sup>4</sup>, Artem Rudenko<sup>9</sup>, Michael Meyer<sup>3,4</sup>, Robin Santra<sup>1,2,3,5</sup>, Ludger Inhester<sup>1,3\*</sup>, Till Jahnke<sup>4,11\*</sup>

# Imaging of small quantum systems



## Equilibrium

- ground state structure
- ground state (quantum, thermal) fluctuations

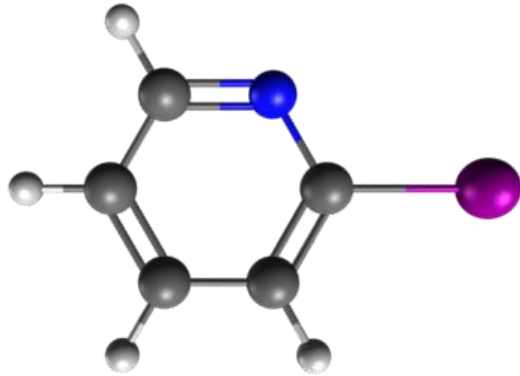
## Out-of-equilibrium (perturbative)

- reactions with environment
- nuclei and electron dynamics (adiabatic and non-adiabatic)
- photo-excitation (photo-cycle)
- coherent control

## Out-of-equilibrium (non-perturbative)

- strong-field ionization
- light-matter states
- strong-field control

# Imaging via x-ray induced Coulomb explosion

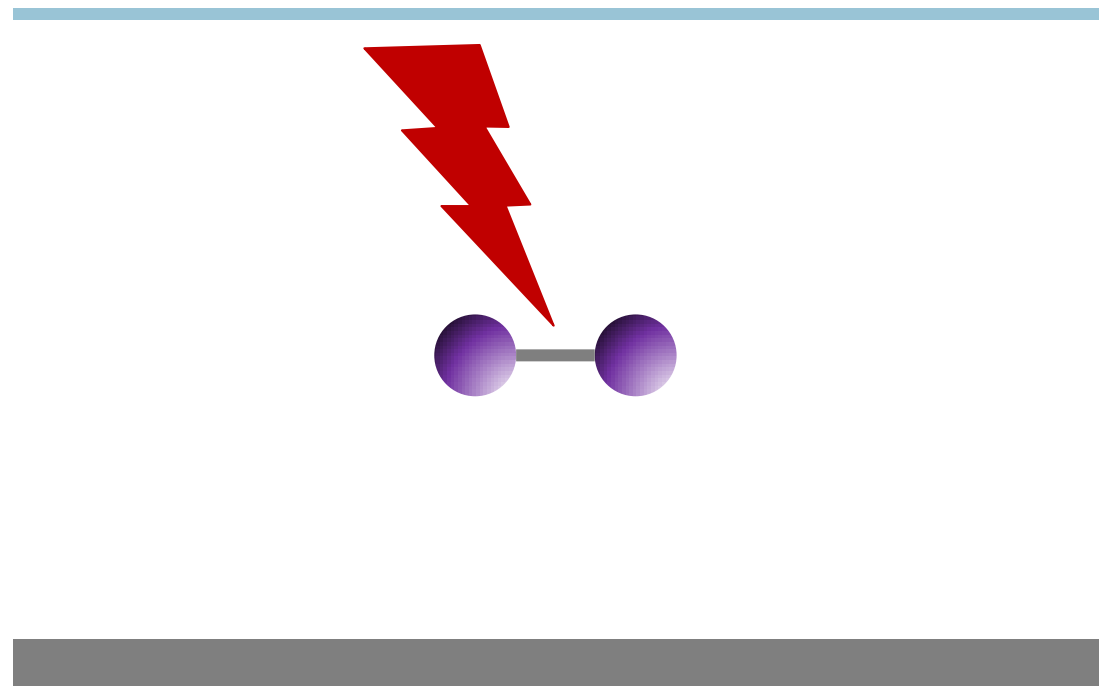


- Has been done before with molecules transiting thin foils or intense ultrafast laser systems
- Destroys the quantum system to retrieve structure
- Retrieving structure from individual 3d momenta of all ions
- X-rays strip electrons from all atoms
- Challenge is to charge molecule before it can do anything else

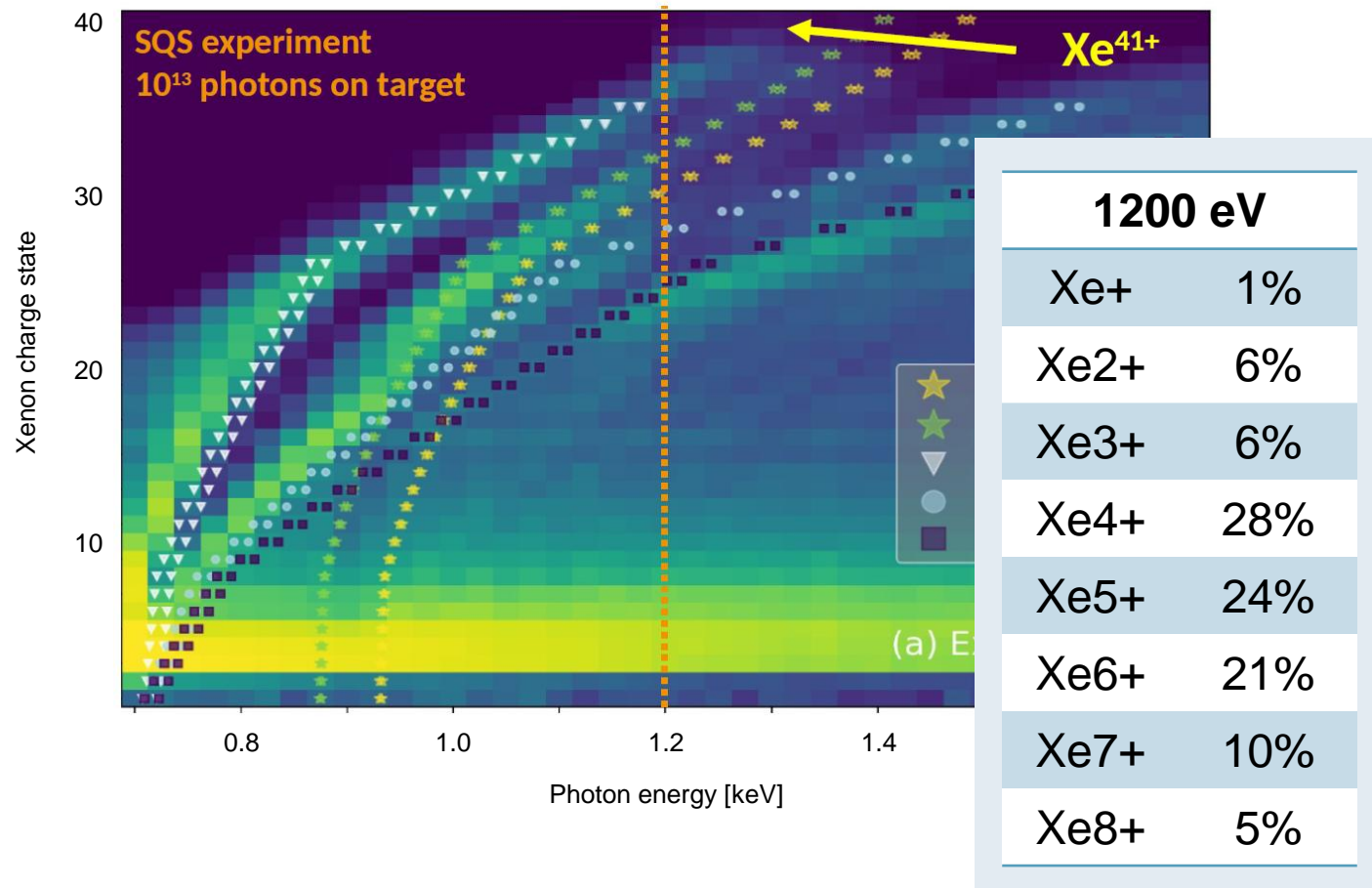


X-ray Free Electron Laser

# X-ray induced Coulomb explosion

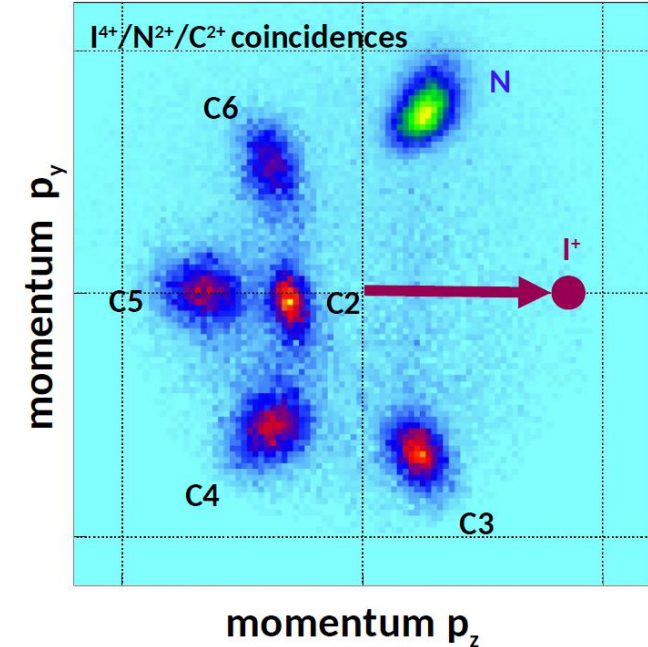
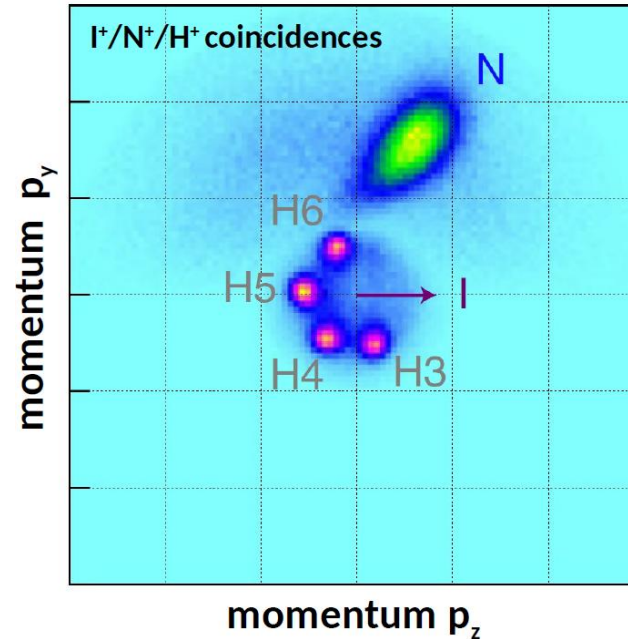
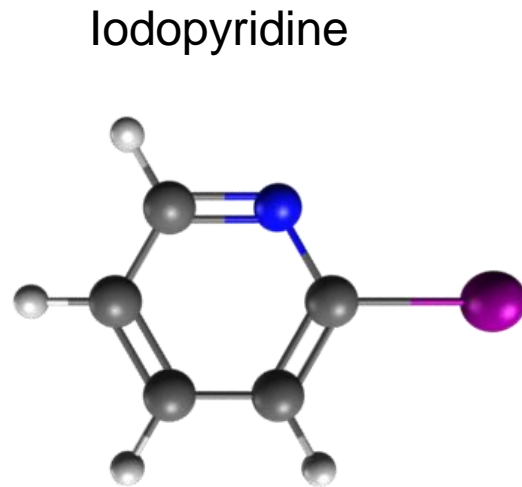


# Intense x-ray pulses



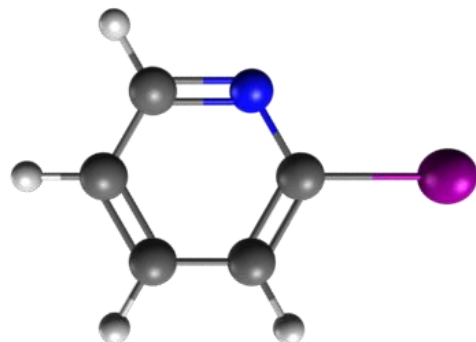
- Very highly charged states via multiple inner-shell processes
- Up to > 40 photons are absorbed with up to 6 core holes generated simultaneously

# Coulomb explosion imaging – CEI

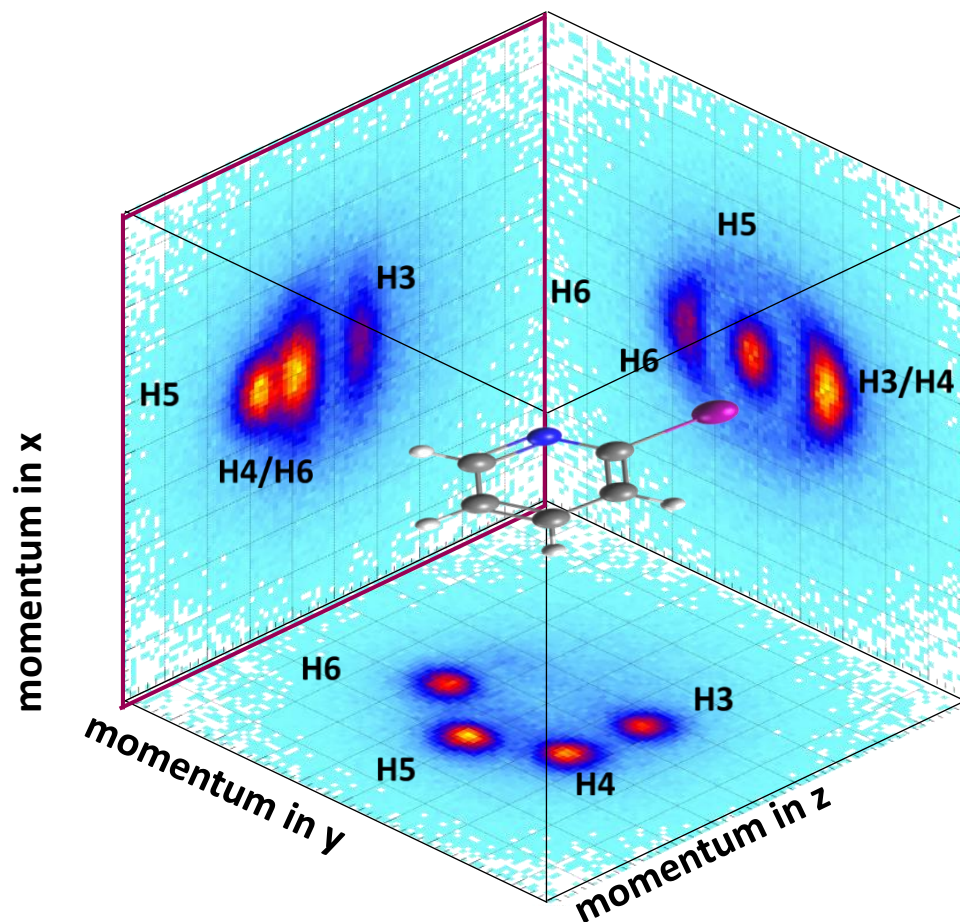


- molecular structure is very well reflected in measured momenta
- no evidence of deformation or rotation before breakup
- 3-fold ion coincidences are sufficient to image the entire molecule
- CEI has the same sensitivity for hydrogen as for any other species – contrary to diffraction methods

# Imaging collective quantum fluctuations of the structure of a complex molecule

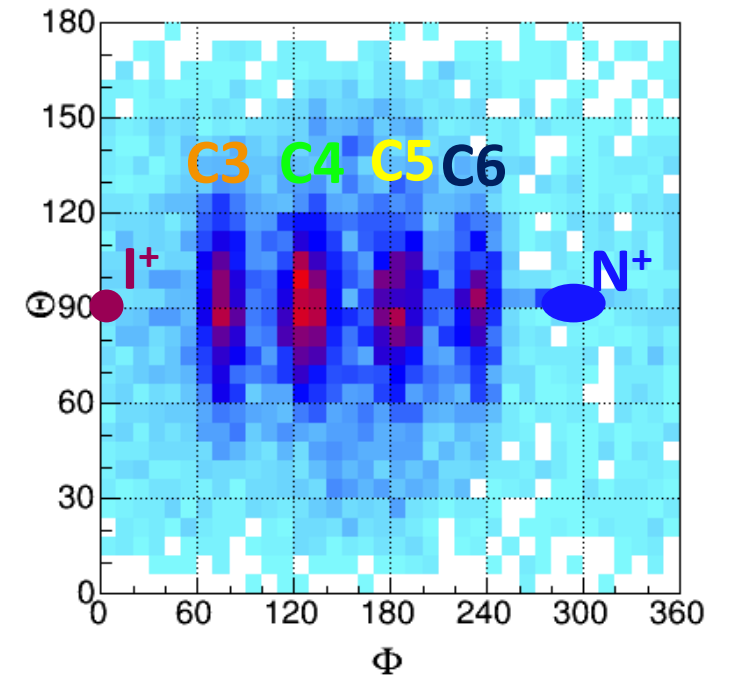
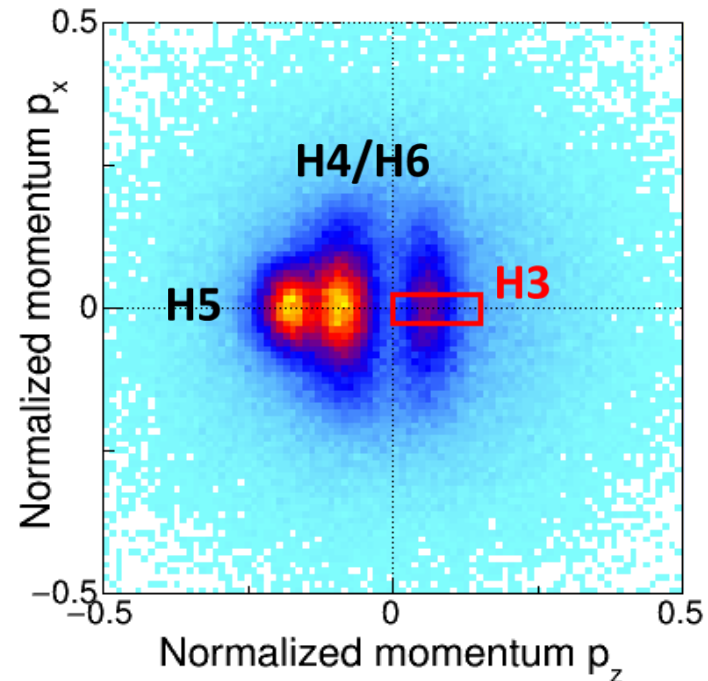


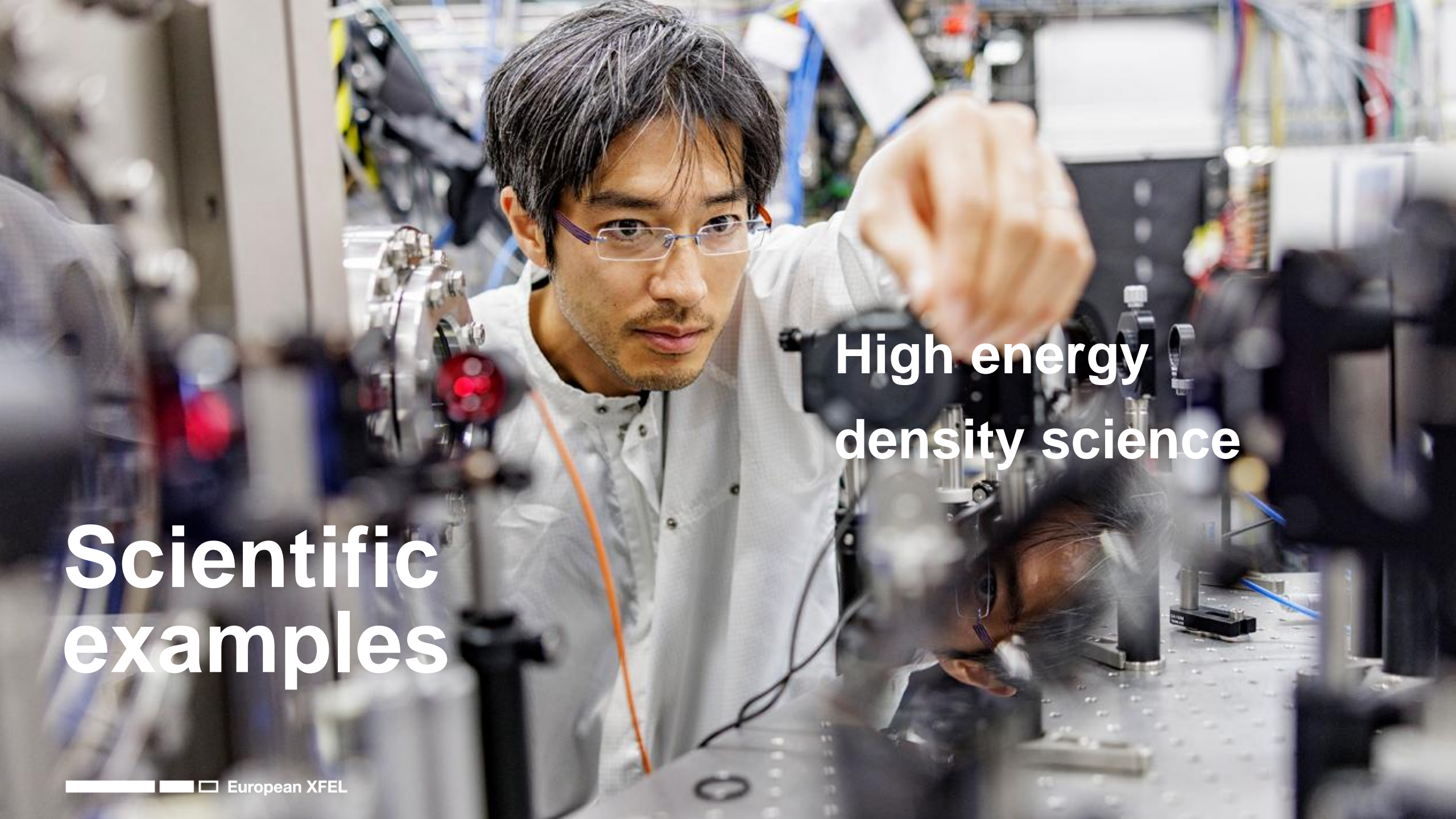
- Even in the ground state molecules are not static but undergo collective structural motions
- These motions are extremely small, but momentum imaging is an exquisitely sensitive tool to observe such small motions



# Imaging collective quantum fluctuations of the structure of a complex molecule

- The emission directions of the atoms are correlated
- Coincidence analysis reveals correlations of the emission directions of hydrogen and carbon atoms perpendicular to the iodine and nitrogen momenta which result from ground state fluctuations





**High energy  
density science**

**Scientific  
examples**

## Observation of Body-Centered Cubic Iron above 200 Gigapascals.

Zuzana Konôpková,<sup>1,\*</sup> Eric Edmund,<sup>2,†</sup> Orianna B Ball,<sup>3</sup> Agnès Dewaele,<sup>4,5</sup> Hélène Ginestet,<sup>6</sup> Rachel J Husband,<sup>7</sup> Nicolas Jaisle,<sup>8</sup> Cornelius Strohm,<sup>7</sup> Madden S Anae,<sup>9</sup> Daniele Antonangeli,<sup>10</sup> Karen Appel,<sup>1</sup> Marzena Baron,<sup>11</sup> Silvia Boccato,<sup>10</sup> Khachiwan Buakor,<sup>1</sup> Julien Chantel,<sup>6</sup> Hyunchae Cynn,<sup>12</sup> Anand P Dwivedi,<sup>1</sup> Lars Ehm,<sup>9</sup> Konstantin Glazyrin,<sup>7</sup> Heinz Graafsma,<sup>7</sup> Egor Koemets,<sup>13,14</sup> Torsten Laurus,<sup>7</sup> Hauke Marquardt,<sup>13</sup> Bernhard Massani,<sup>3</sup> James D McHardy,<sup>3</sup> Malcolm I McMahon,<sup>3</sup> Vitali Prakapenka,<sup>15</sup> Jolanta Sztuk-Dambietz,<sup>1</sup> Minxue Tang,<sup>7</sup> Tianqi Xie,<sup>9,16</sup> Zena Younes,<sup>3</sup> Ulf Zastrau,<sup>1</sup> Alexander F Goncharov,<sup>2</sup> Clemens Prescher,<sup>17</sup> Ryan S McWilliams,<sup>3</sup> Guillaume Morard,<sup>8,10</sup> and Sébastien Merkel<sup>6</sup>

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### Phase transition kinetics of superionic H<sub>2</sub>O ice phases revealed by Megahertz X-ray free-electron laser-heating experiments

[R. J. Husband](#) , [H. P. Liermann](#), [J. D. McHardy](#), [R. S. McWilliams](#), [A. F. Goncharov](#), [V. B.](#)

[Prakapenka](#), [E. Edmund](#), [S. Chariton](#), [Z. Konôpková](#), [C. Strohm](#), [C. Sanchez-Valle](#), [M. Frost](#), [L. Andriambariarijaona](#), [K. Appel](#), [C. Baehtz](#), [O. B. Ball](#), [R. Briggs](#), [J. Buchen](#), [V. Cerantola](#), [J. Choi](#), [A. L. Coleman](#), [H. Cynn](#), [A. Dwivedi](#), [H. Graafsma](#), [H. Hwang](#), [E. Koemets](#), [T. Laurus](#), [Y. Lee](#), [X. Li](#), [H. Marquardt](#), [A. Mondal](#), [M. Nakatsutsumi](#), [S. Ninet](#), [E. Pace](#), [C. Pepin](#), [C. Prescher](#), [S. Stern](#), [J. Sztuk-Dambietz](#), [U. Zastrau](#) & [M. I. McMahon](#) 

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Article

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### Diamond precipitation dynamics from hydrocarbons at icy planet interior conditions

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 Check for updates

Mungo Frost<sup>1,✉</sup>, R. Stewart McWilliams<sup>2</sup>, Elena Bykova<sup>3</sup>, Maxim Bykov<sup>4</sup>, Rachel J. Husband<sup>5</sup>, Leon M. Andriambariarijaona<sup>6</sup>, Saiana Khandarkhaeva<sup>6</sup>, Bernhard Massani<sup>7</sup>, Karen Appel<sup>7</sup>, Carsten Baehtz<sup>8</sup>, Orianna B. Ball<sup>2</sup>, Valerio Cerantola<sup>7</sup>, Stella Chariton<sup>9</sup>, Jinhyuk Choi<sup>10</sup>, Hyunchae Cynn<sup>11</sup>, Matthew J. Duff<sup>2</sup>, Anand Dwivedi<sup>12</sup>, Eric Edmund<sup>13</sup>, Guillaume Fiquet<sup>6</sup>, Heinz Graafsma<sup>14</sup>, Huijeong Hwang<sup>15</sup>, Nicolas Jaisle<sup>16</sup>, Jaeyong Kim<sup>15</sup>, Zuzana Konôpková<sup>7</sup>, Torsten Laurus<sup>17</sup>, Yongjae Lee<sup>10</sup>, Hanns-Peter Liermann<sup>18</sup>, James D. McHardy<sup>19</sup>, Malcolm I. McMahon<sup>20</sup>, Guillaume Morard<sup>21</sup>, Motoaki Nakatsutsumi<sup>22</sup>, Lan Anh Nguyen<sup>15</sup>, Sandra Ninet<sup>23</sup>, Vitali B. Prakapenka<sup>24</sup>, Clemens Prescher<sup>25</sup>, Ronald Redmer<sup>26</sup>, Stephan Stern<sup>27,28,29</sup>, Cornelius Strohm<sup>30</sup>, Jolanta Sztuk-Dambietz<sup>31</sup>, Monica Turcato<sup>32</sup>, Zhongyan Wu<sup>33</sup>, Siegfried H. Glenzer<sup>34</sup> & Alexander F. Goncharov<sup>35</sup>

## Article

### The structure of liquid carbon elucidated by in situ X-ray diffraction

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D. Kraus<sup>1,2,✉</sup>, J. Rips<sup>1</sup>, M. Schörner<sup>1</sup>, M. G. Stevenson<sup>1</sup>, J. Vorberger<sup>2</sup>, D. Ranjan<sup>1,2</sup>, J. Lüttgert<sup>1</sup>, B. Heuser<sup>1</sup>, J. H. Eggert<sup>3</sup>, H.-P. Liermann<sup>4</sup>, I. I. Oleynik<sup>5</sup>, S. Pandolfi<sup>6</sup>, R. Redmer<sup>1</sup>, A. Sollier<sup>7,8</sup>, C. Strohm<sup>4</sup>, T. J. Volz<sup>3</sup>, B. Albertazzi<sup>9</sup>, S. J. Ali<sup>2</sup>, L. Antonelli<sup>10</sup>, C. Bächtz<sup>2</sup>, O. B. Ball<sup>11</sup>, S. Banerjee<sup>12</sup>, A. B. Belonoshko<sup>13</sup>, C. A. Bolme<sup>14</sup>, V. Bouffetier<sup>15</sup>, R. Briggs<sup>3</sup>, K. Buakor<sup>16</sup>, T. Butcher<sup>12</sup>, V. Cerantola<sup>10</sup>, J. Chantel<sup>17</sup>, A. L. Coleman<sup>18</sup>, J. Collier<sup>12</sup>, G. W. Collins<sup>19,20</sup>, A. J. Comley<sup>21</sup>, T. E. Cowan<sup>2</sup>, G. Cristoforetti<sup>22</sup>, H. Cynn<sup>23</sup>, A. Descamps<sup>23</sup>, A. Di Cicco<sup>24</sup>, S. Di Dio Cafiso<sup>2</sup>, F. Dorchie<sup>25</sup>, M. J. Duff<sup>1</sup>, A. Dwivedi<sup>15</sup>, C. Edwards<sup>12</sup>, D. Errandonea<sup>26</sup>, S. Galitskiy<sup>5</sup>, E. Galtier<sup>27</sup>, H. Ginestet<sup>17</sup>, L. Gizzi<sup>22</sup>, A. Gleason<sup>27</sup>, S. Göde<sup>15</sup>, J. M. Gonzalez<sup>5</sup>, M. G. Gorman<sup>2,28</sup>, M. Harmand<sup>29,30</sup>, N. J. Hartley<sup>27</sup>, P. G. Heighway<sup>31</sup>, C. Hernandez-Gomez<sup>12</sup>, A. Higginbotham<sup>10</sup>, H. Höppner<sup>2</sup>, R. J. Husband<sup>2</sup>, T. M. Hutchinson<sup>3</sup>, H. Hwang<sup>4,32</sup>, D. A. Keen<sup>33</sup>, J. Kim<sup>34</sup>, P. Koester<sup>35</sup>, Z. Konôpková<sup>15</sup>, A. Krygier<sup>3</sup>, L. Labate<sup>35</sup>, A. Laso Garcia<sup>3</sup>, A. E. Lazicki<sup>3</sup>, Y. Lee<sup>36</sup>, P. Mason<sup>12</sup>, M. Masruri<sup>2</sup>, B. Massani<sup>11</sup>, E. E. McBride<sup>23</sup>, J. D. McHardy<sup>11</sup>, D. McGonigle<sup>21</sup>, C. McGuire<sup>3</sup>, R. S. McWilliams<sup>11</sup>, S. Merkel<sup>17</sup>, G. Morard<sup>17</sup>, B. Nagler<sup>27</sup>, M. Nakatsutsumi<sup>15</sup>, K. Nguyen-Cong<sup>3</sup>, A.-M. Norton<sup>10</sup>, N. Ozaki<sup>30</sup>, C. Otzen<sup>30</sup>, D. J. Peake<sup>31</sup>, A. Pelka<sup>2</sup>, K. A. Pereira<sup>40</sup>, J. P. Phillips<sup>12</sup>, C. Prescher<sup>30</sup>, T. R. Preston<sup>15</sup>, L. Randolph<sup>15</sup>, A. Ravasio<sup>9</sup>, D. Santamaria-Perez<sup>26</sup>, D. J. Savage<sup>14</sup>, M. Schölermerich<sup>41</sup>, J.-P. Schwinkendorf<sup>2</sup>, S. Singh<sup>3</sup>, J. Smith<sup>12</sup>, R. F. Smith<sup>3</sup>, J. Spear<sup>12</sup>, C. Spindloe<sup>12</sup>, T.-A. Suer<sup>18</sup>, M. Tang<sup>4</sup>, M. Toncian<sup>2</sup>, T. Toncian<sup>2</sup>, S. J. Tracy<sup>42</sup>, A. Trapananti<sup>24</sup>, C. E. Vennari<sup>2</sup>, T. Vinci<sup>2</sup>, M. Tyldesley<sup>2</sup>, S. C. Vogel<sup>14</sup>, J. P. S. Walsh<sup>10</sup>, J. S. Wark<sup>3</sup>, J. T. Willman<sup>5</sup>, L. Wollenweber<sup>15</sup>, U. Zastrau<sup>15</sup>, E. Brambrink<sup>15</sup>, K. Appel<sup>15</sup> & M. I. McMahon<sup>11</sup>

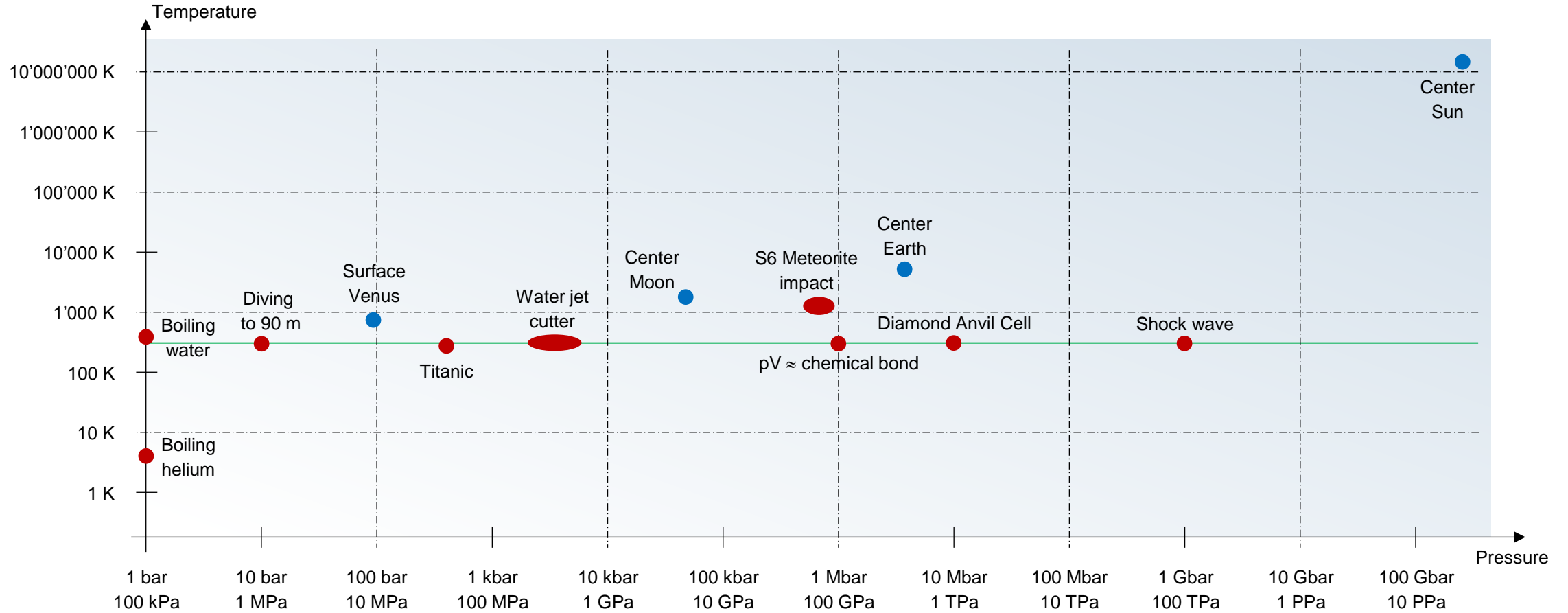


Zuzana Konôpková

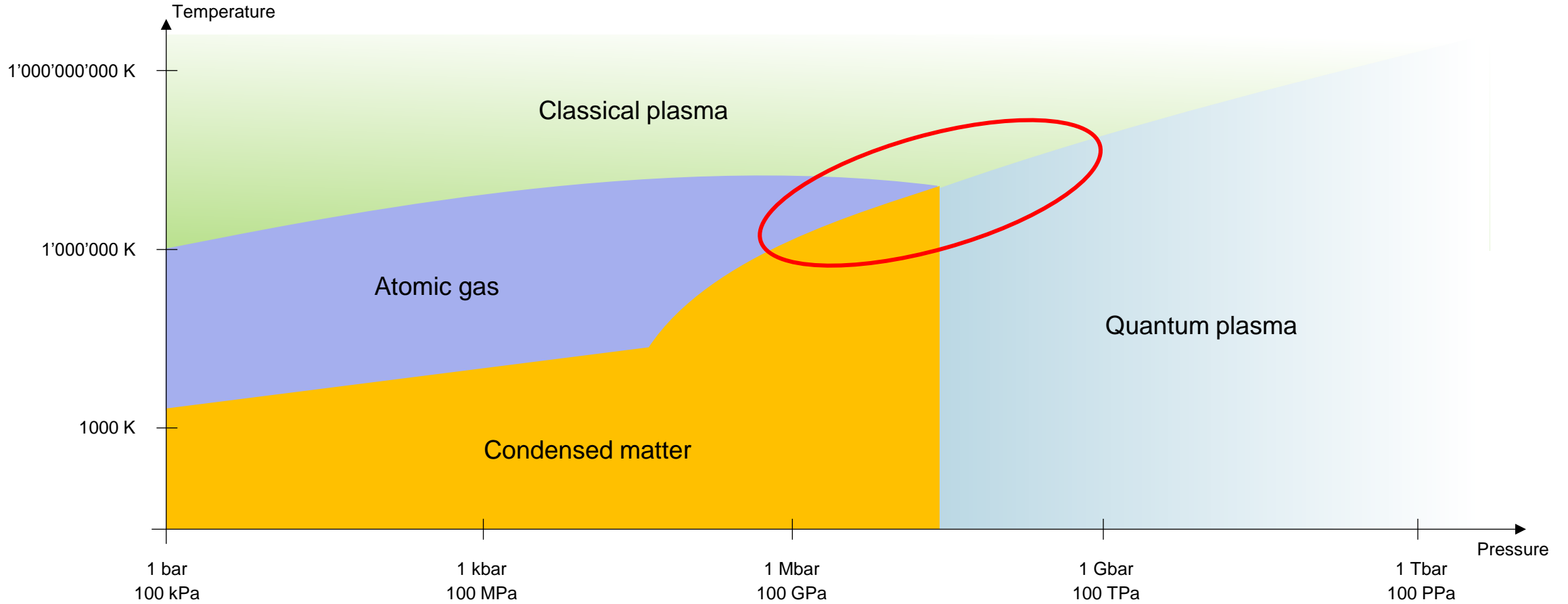


Karen Appel

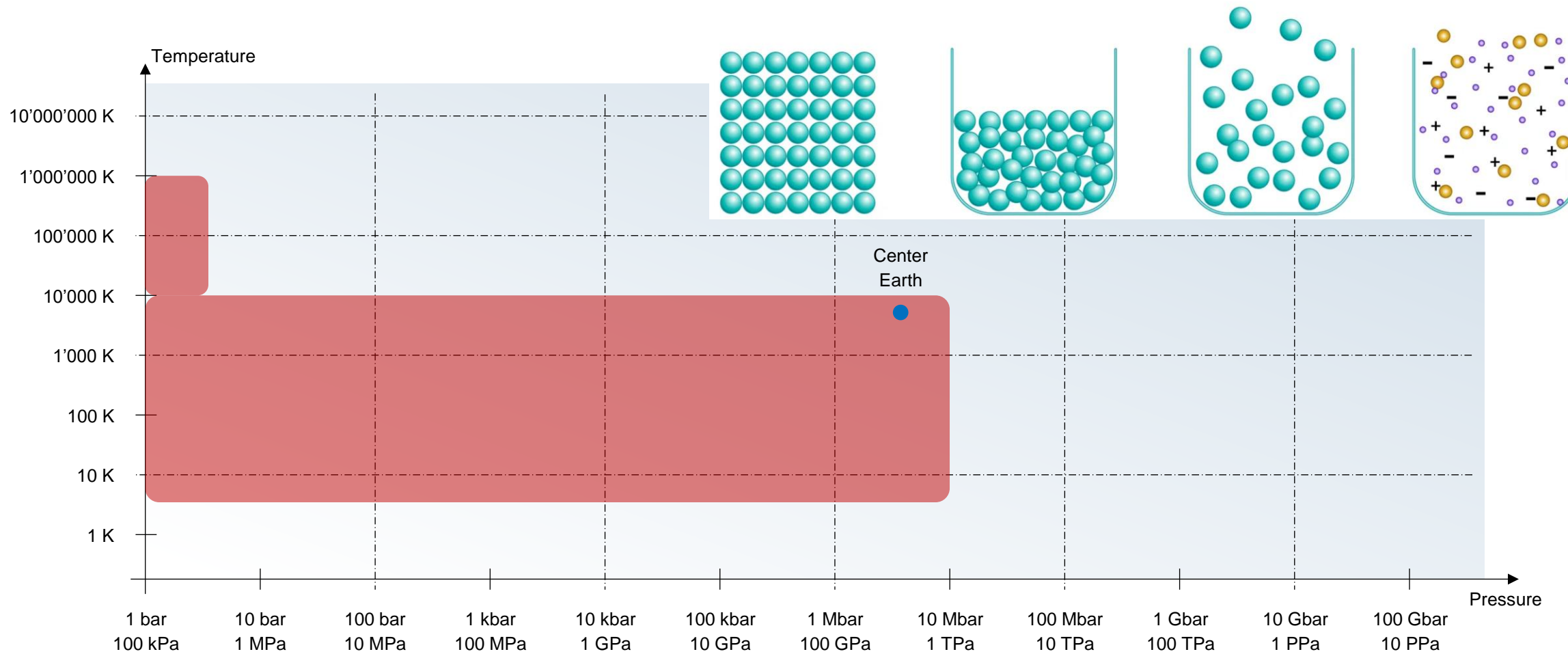
# About pressure and temperature – a phase diagram



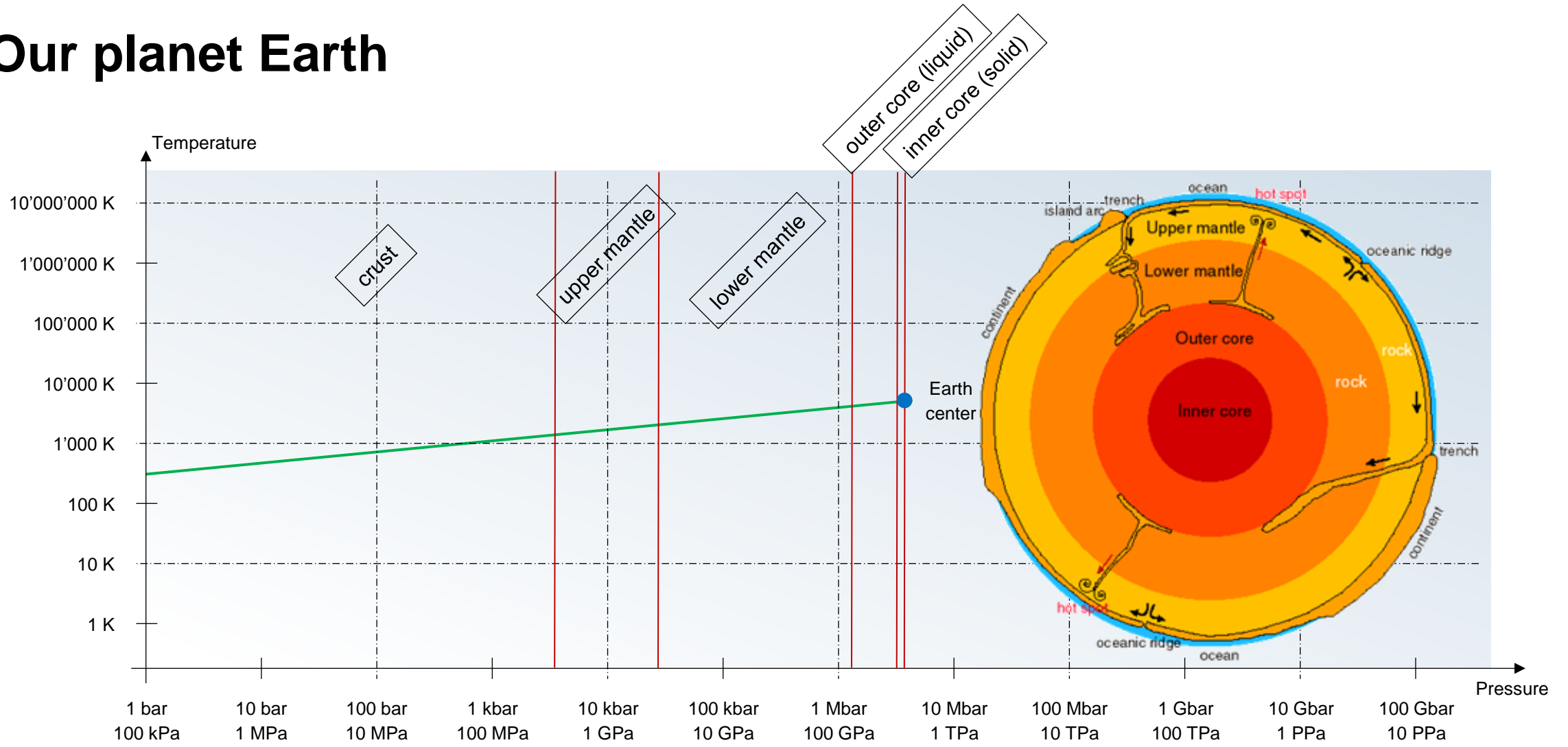
# Warm dense matter



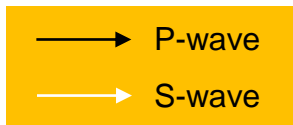
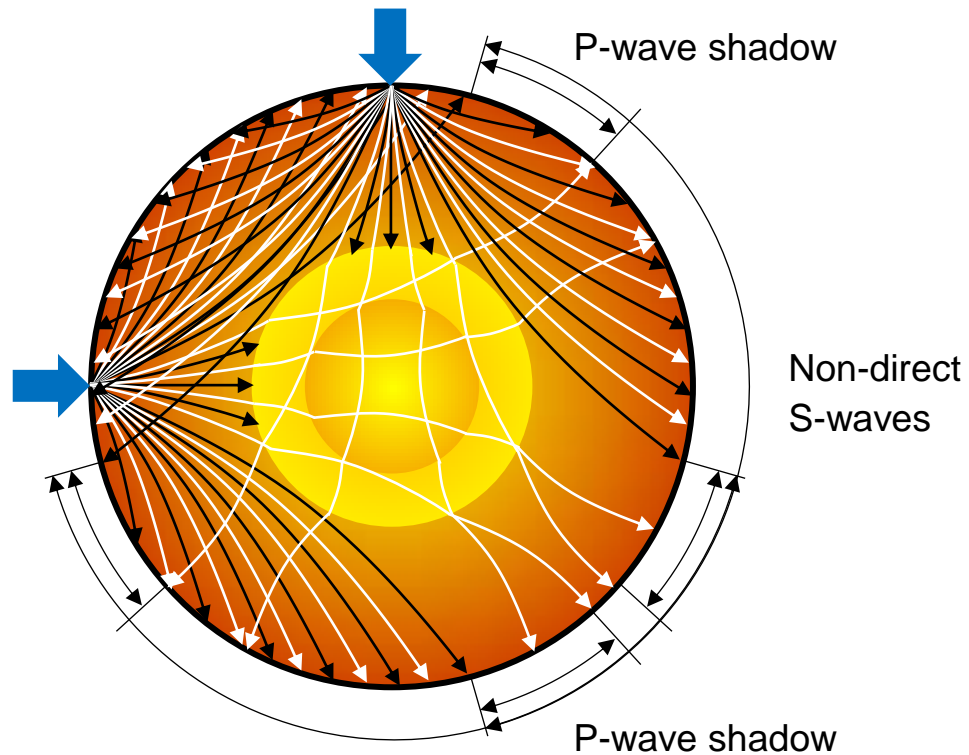
# The power of European XFEL



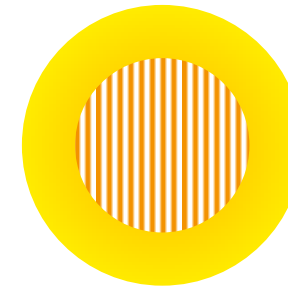
# Our planet Earth



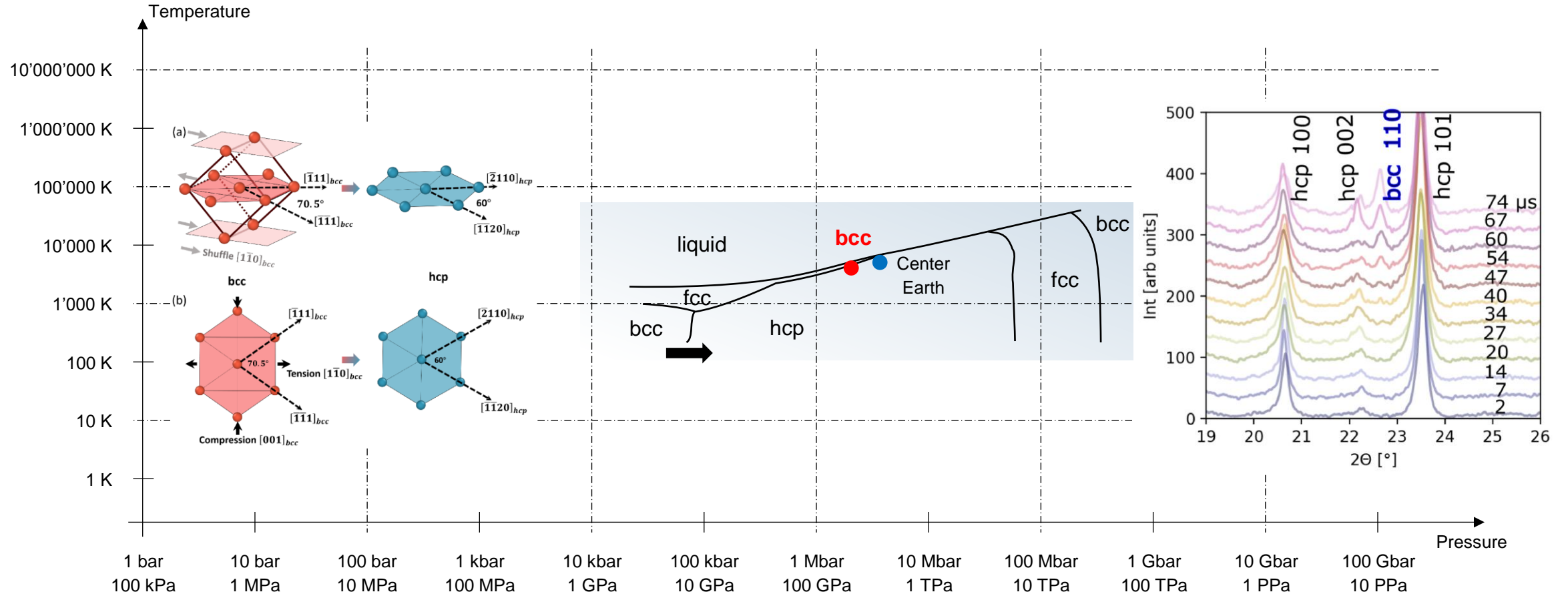
# What do we know about the inner part of Earth



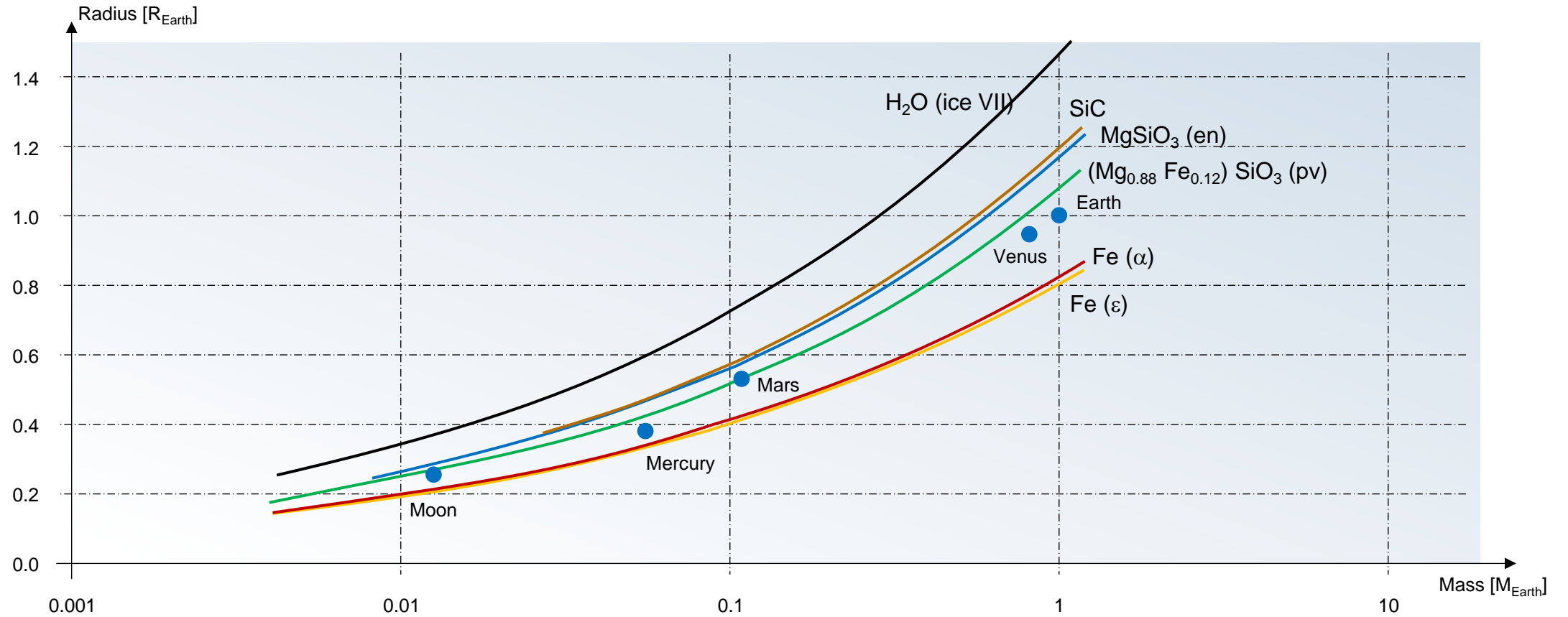
- P-wave shadow:** Solid mantle and liquid core
- Non-direct S-waves:** Liquid outer and solid inner core
- Source at north pole:** Waves travel faster -> Anisotropic inner core



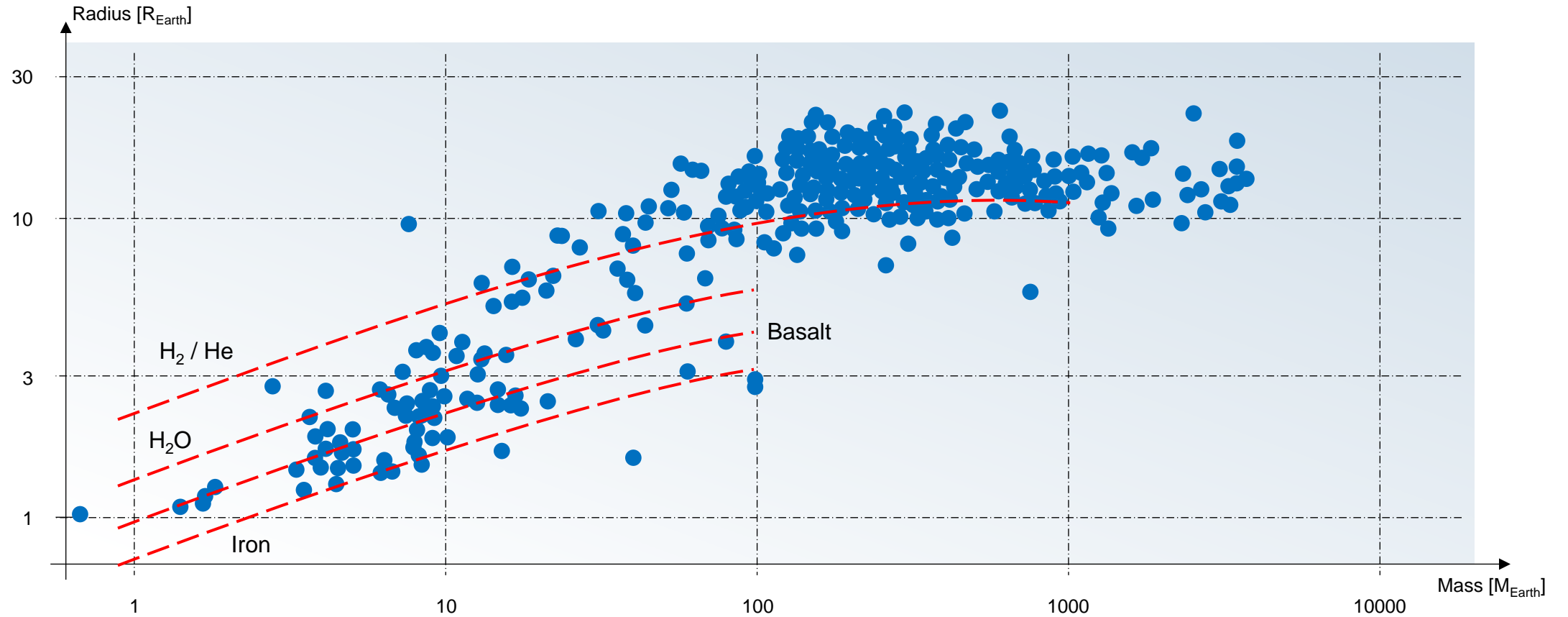
# The phase diagram of Iron



# Rock planets in our solar system

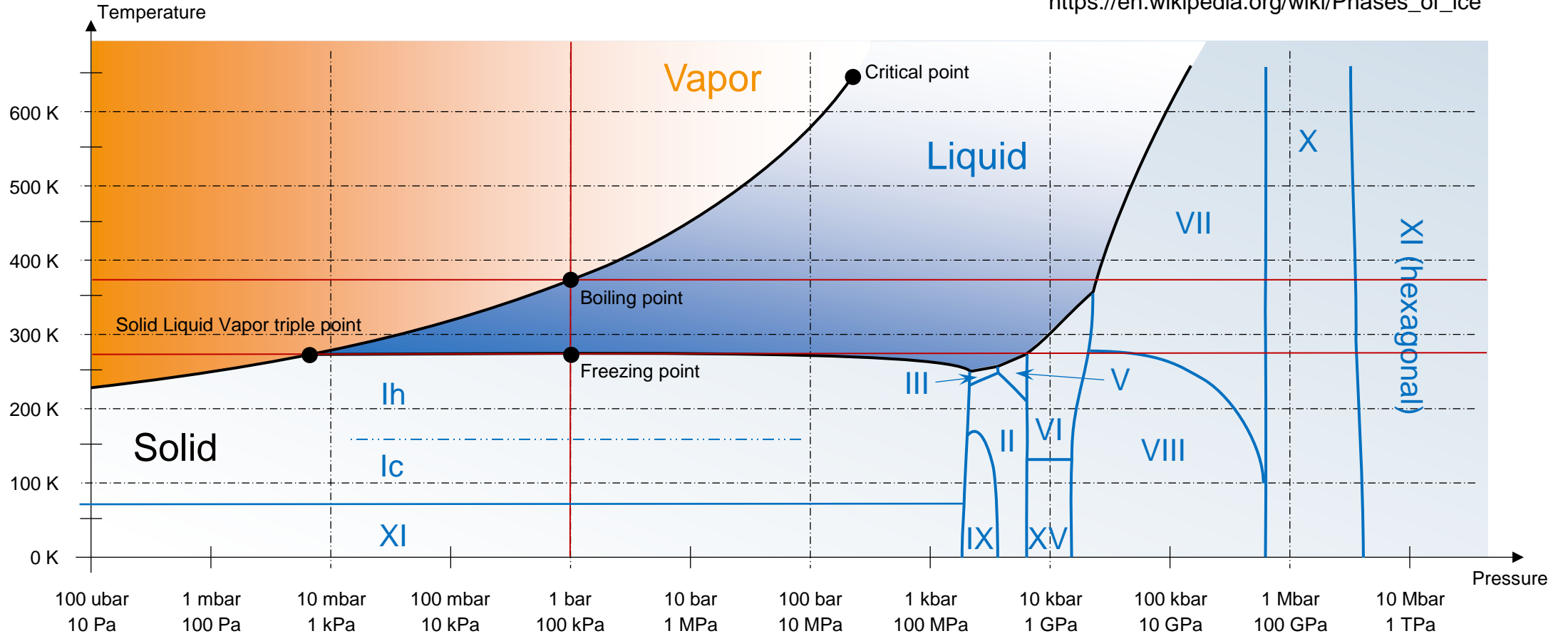


# By now thousands of exoplanets have been discovered

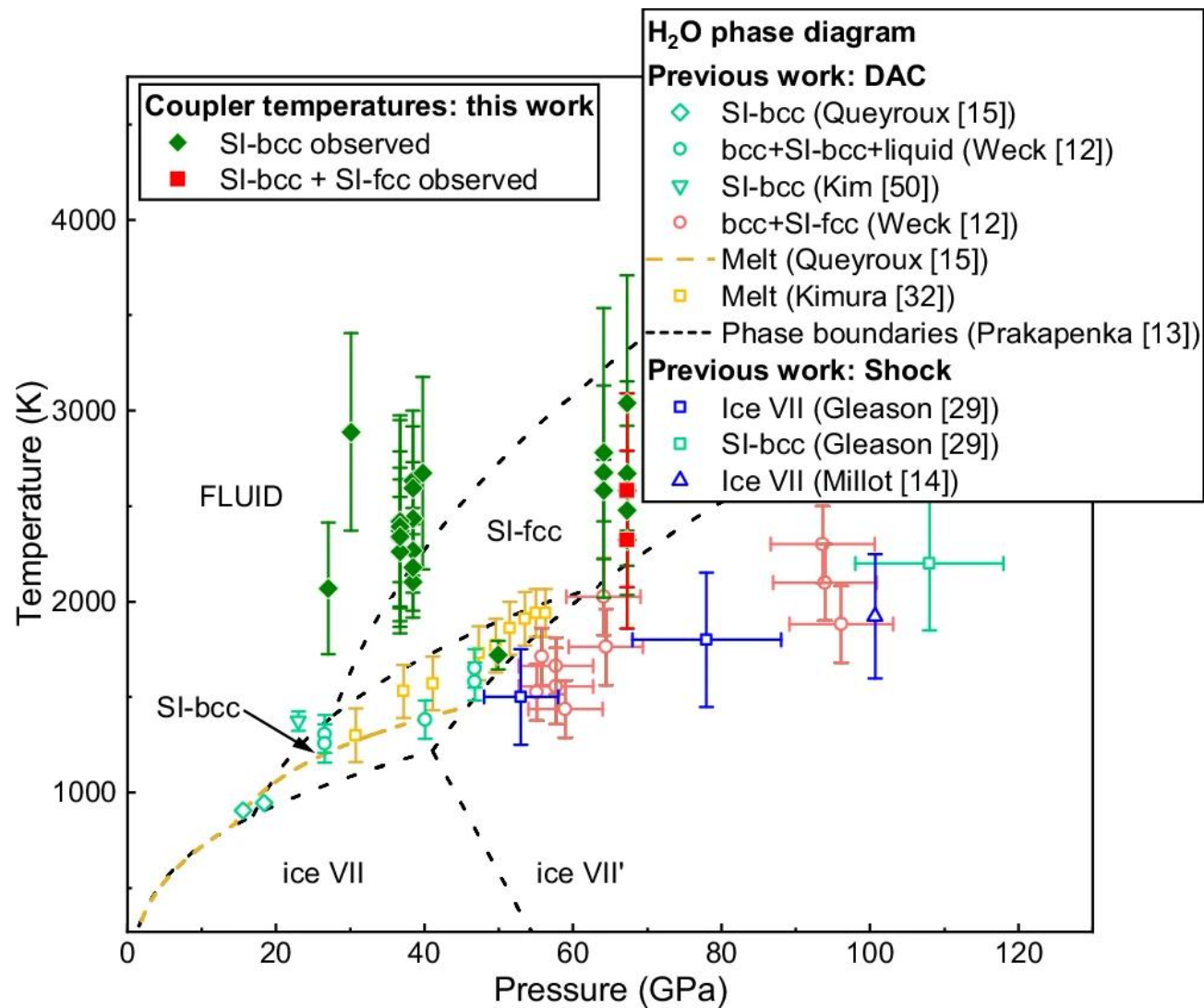
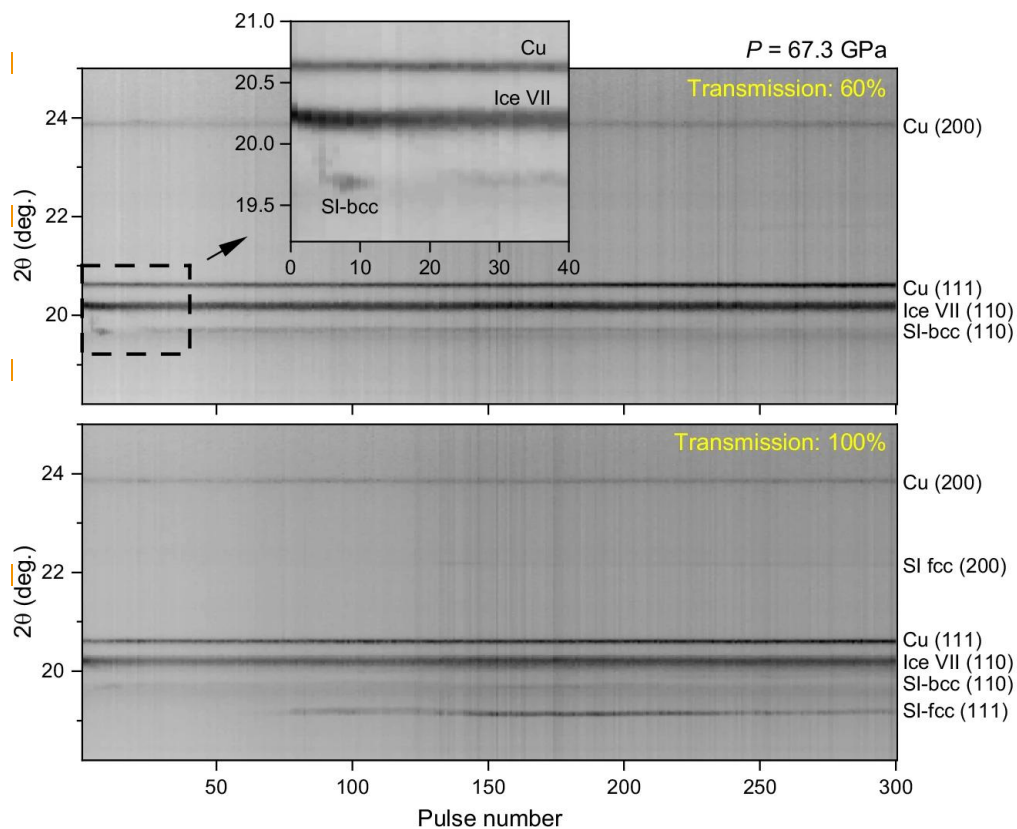


# Phase diagram of water

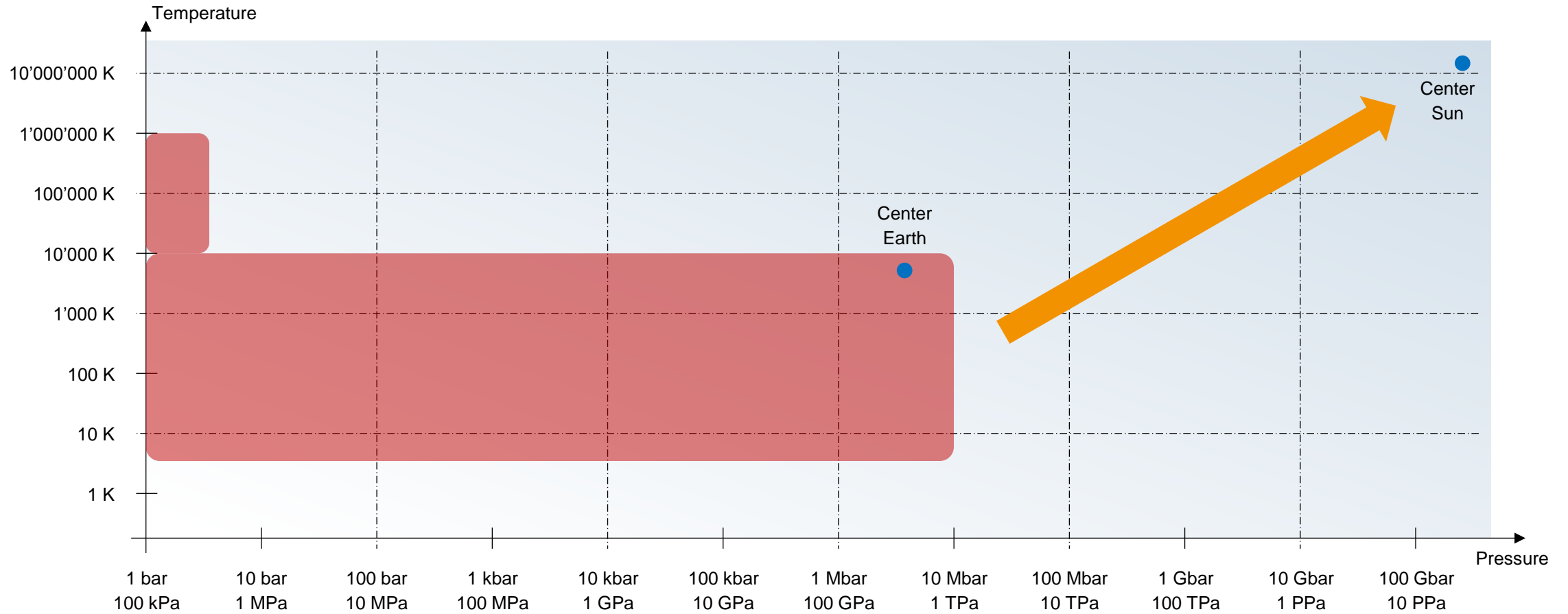
[https://en.wikipedia.org/wiki/Phases\\_of\\_ice](https://en.wikipedia.org/wiki/Phases_of_ice)



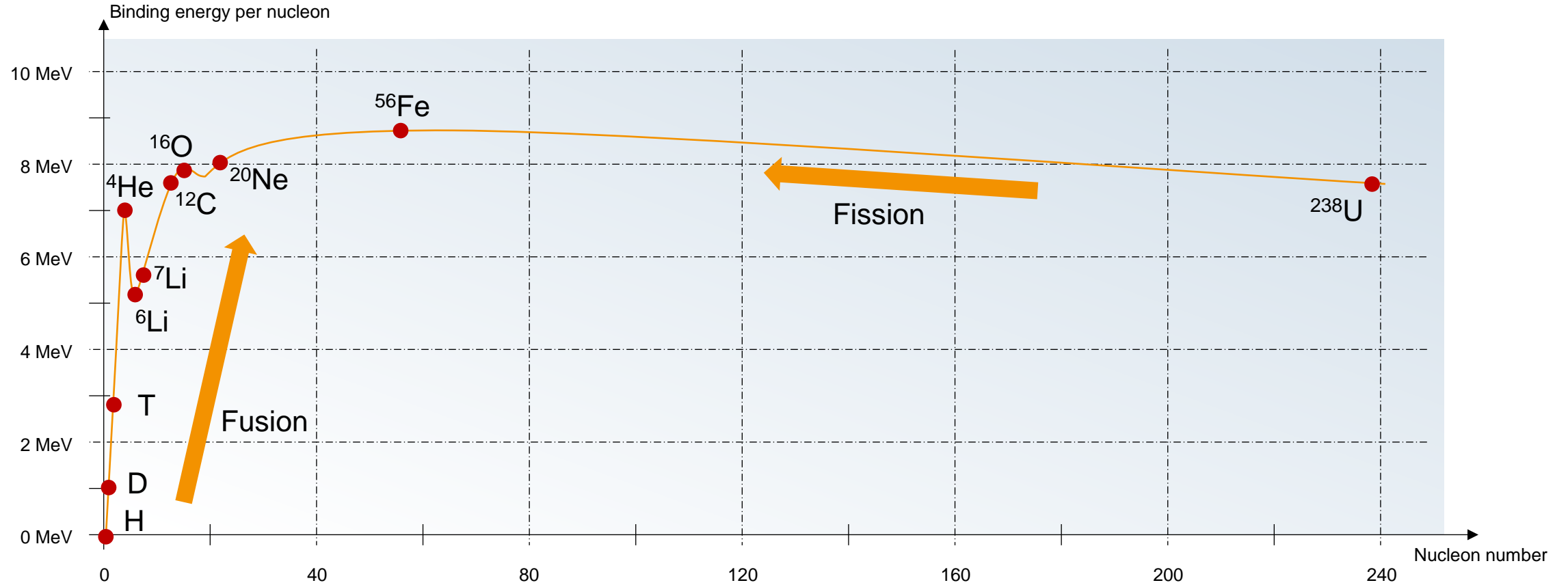
# Phase diagram of water



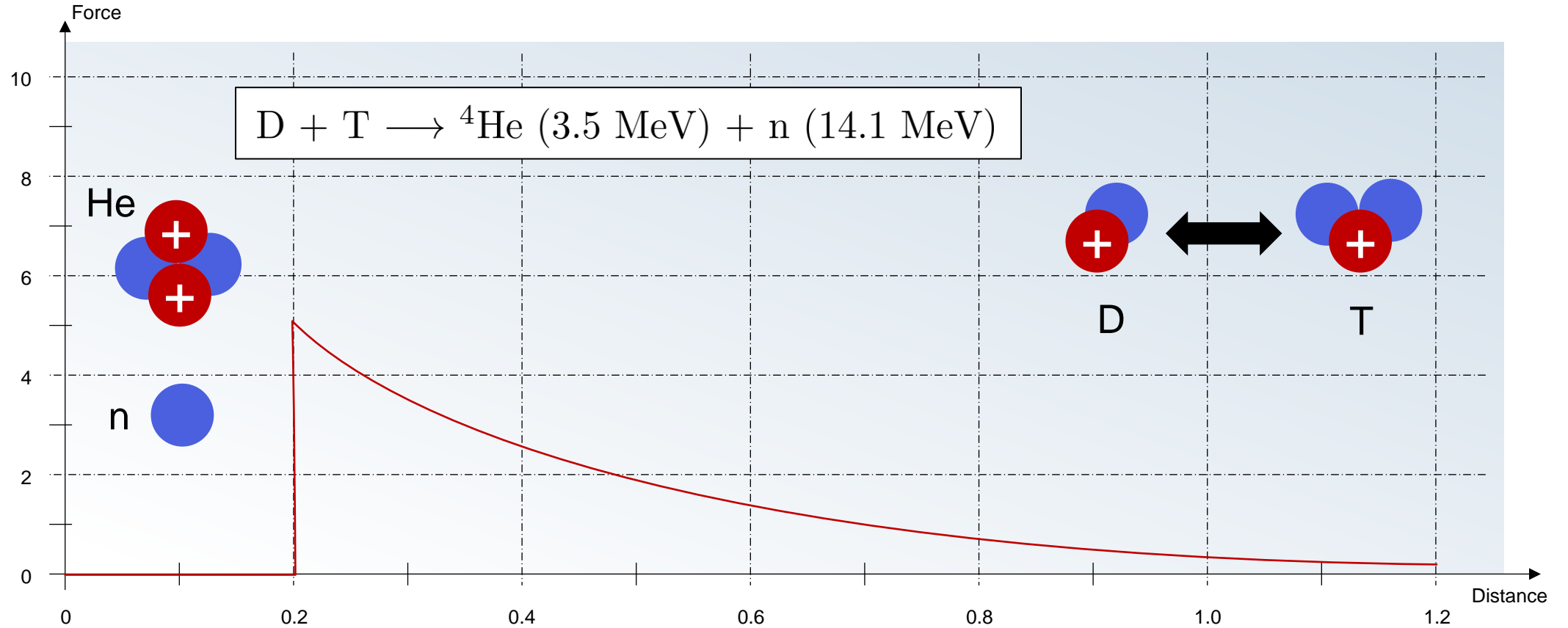
# The center of the Sun



# An excursion to nuclear physics

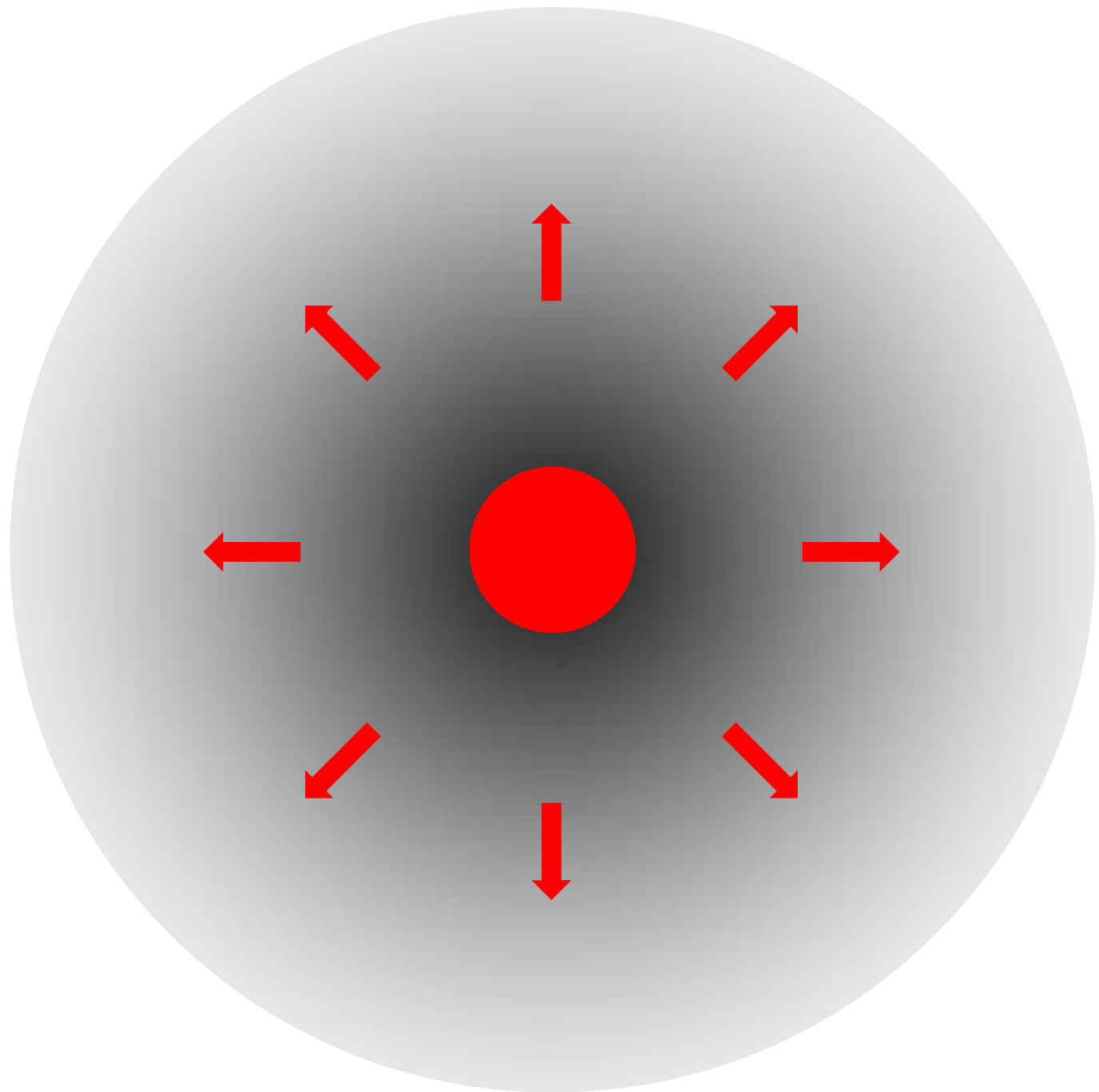


# Overcoming the repulsive Coulomb force



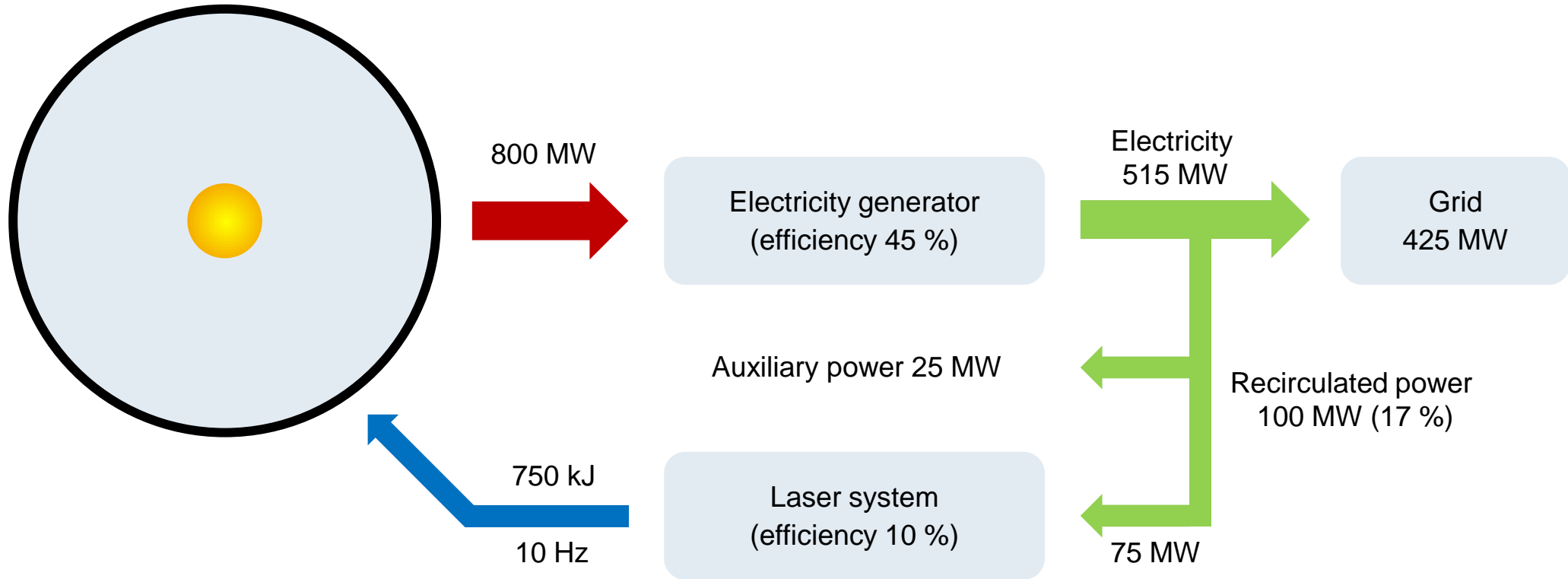
# Building little suns

- European XFEL is the only facility worldwide able to observe the details of this process
- We are committed to contribute to the quest for a new energy source
- Currently, we are discussing with stakeholders and are in the planning phase

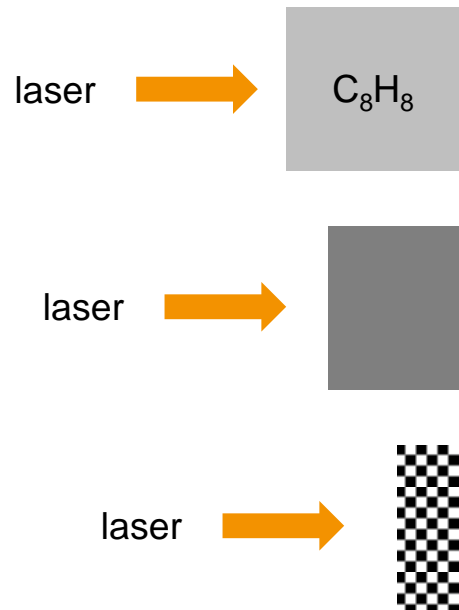


# Electricity budget

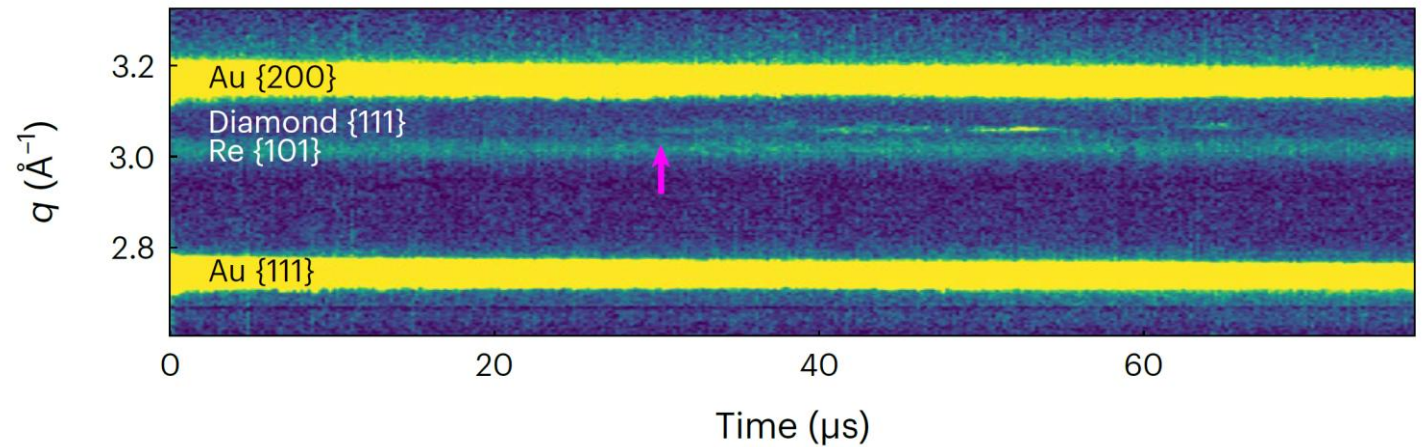
Target gain = 160



# Already the ablator is full of surprises



- Between 19 and 27 GPa: formation of diamond
- Temperature: above 2'500 K for 30 to 40 us



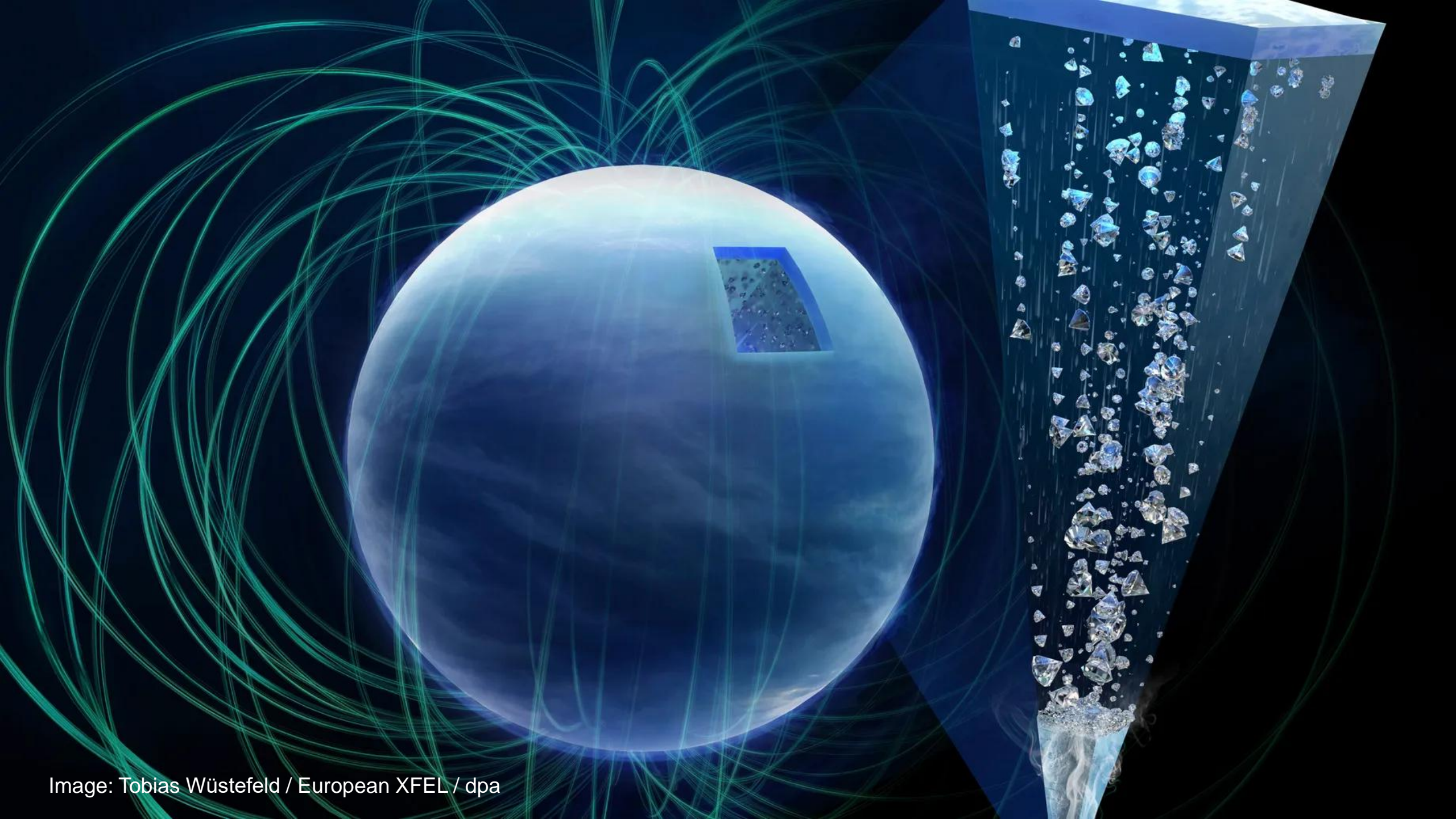
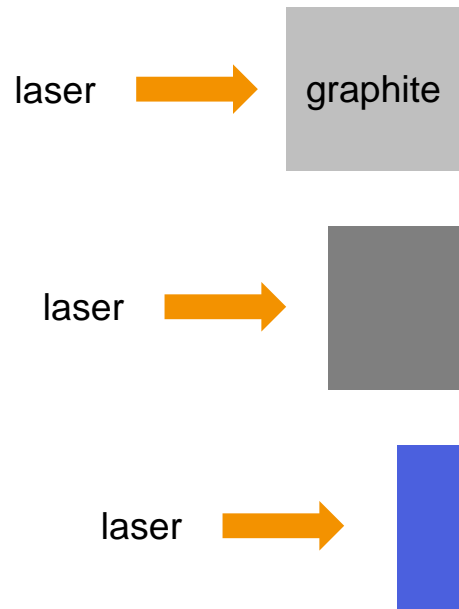


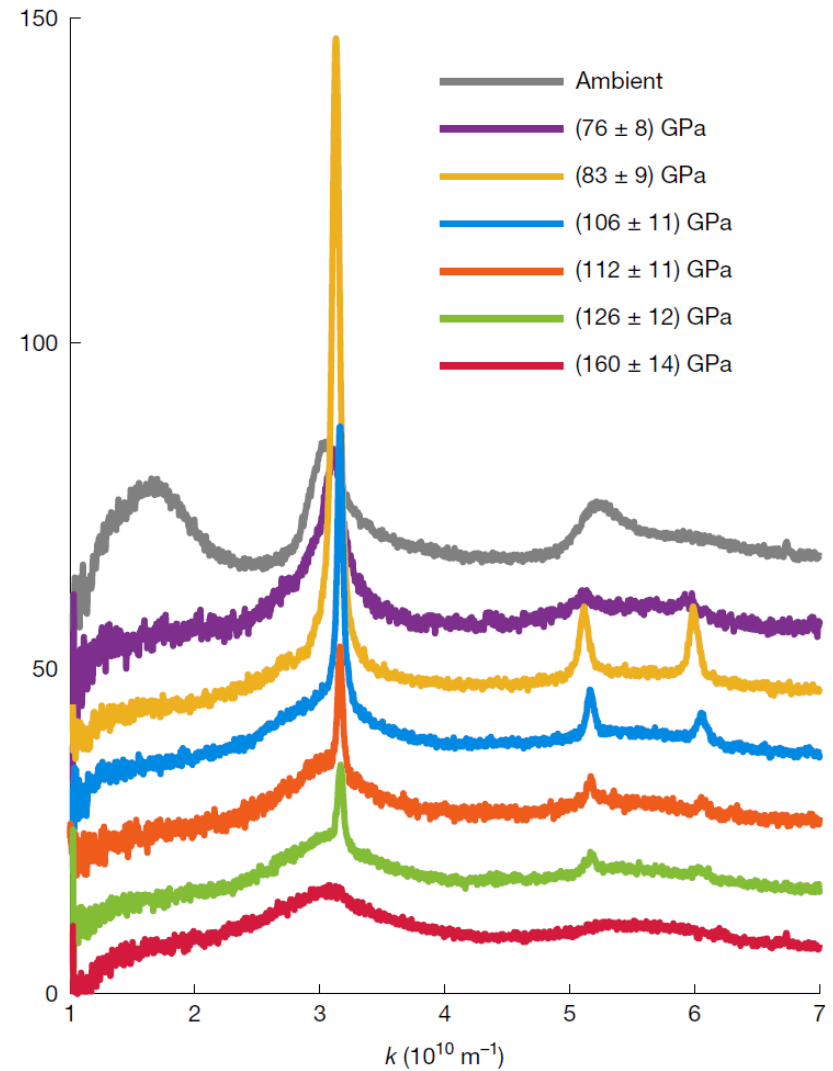
Image: Tobias Wüstefeld / European XFEL / dpa

# The mysterious liquid carbon



■ Above 50 GPa: formation of diamond

■ Above 150 GPa: carbon melts



# Thank you for your attention

