# Evolution of atomic clusters irradiated by short-wavelength FEL radiation

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in collaboration with C. Bostedt (SLAC),
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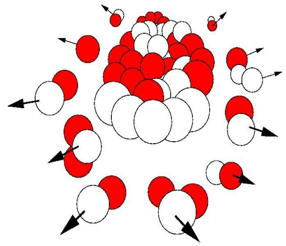
and T. Mőller (TU Berlin)



EMMI Workshop on Plasma Physics, Darmstadt, 2-4 May 2011

HELMHOLTZ ASSOCIATION

CFEL SCIENCE

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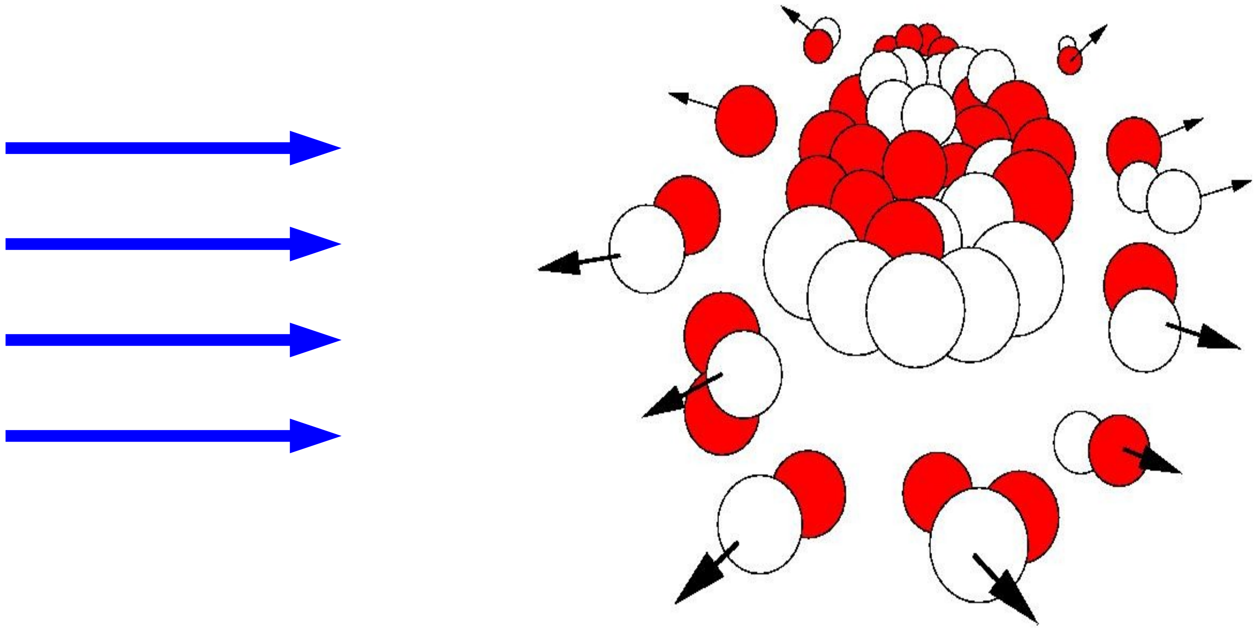
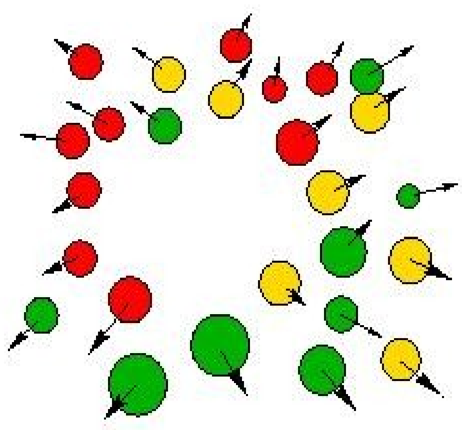
# Motivation for theoretical study

Important for: (i) experiments with FEL → cluster experiments, single particle imaging, warm dense matter etc.
(ii) construction of the laser → FEL optics,
(iii) test of various theoretical models



# Tool: statistical Boltzmann approach

Evolution of larger systems described in terms of statistical density function, ρ(r,v,t), in phase space:



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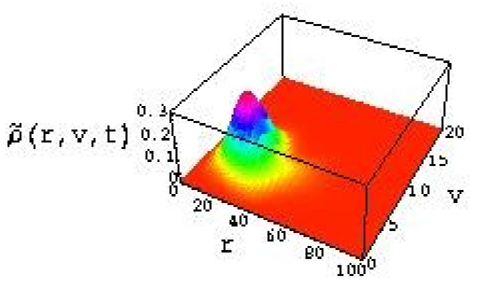
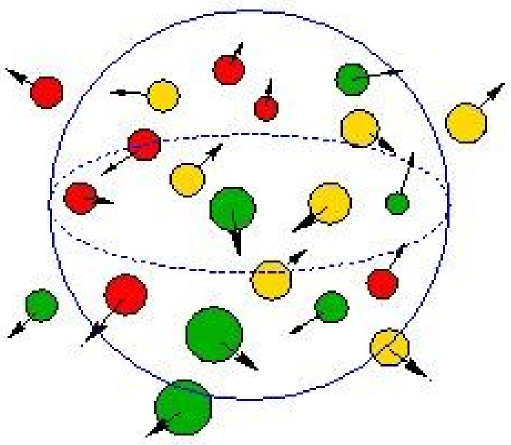


# Tool: statistical Boltzmann approach

- first-principle approach
- single-run method
- computational costs do not scale with number of atoms

Boltzmann equations are able to follow

non-equilibrium processes



Difficulty:

- requires advanced numerical methods

# Solving Boltzmann equations

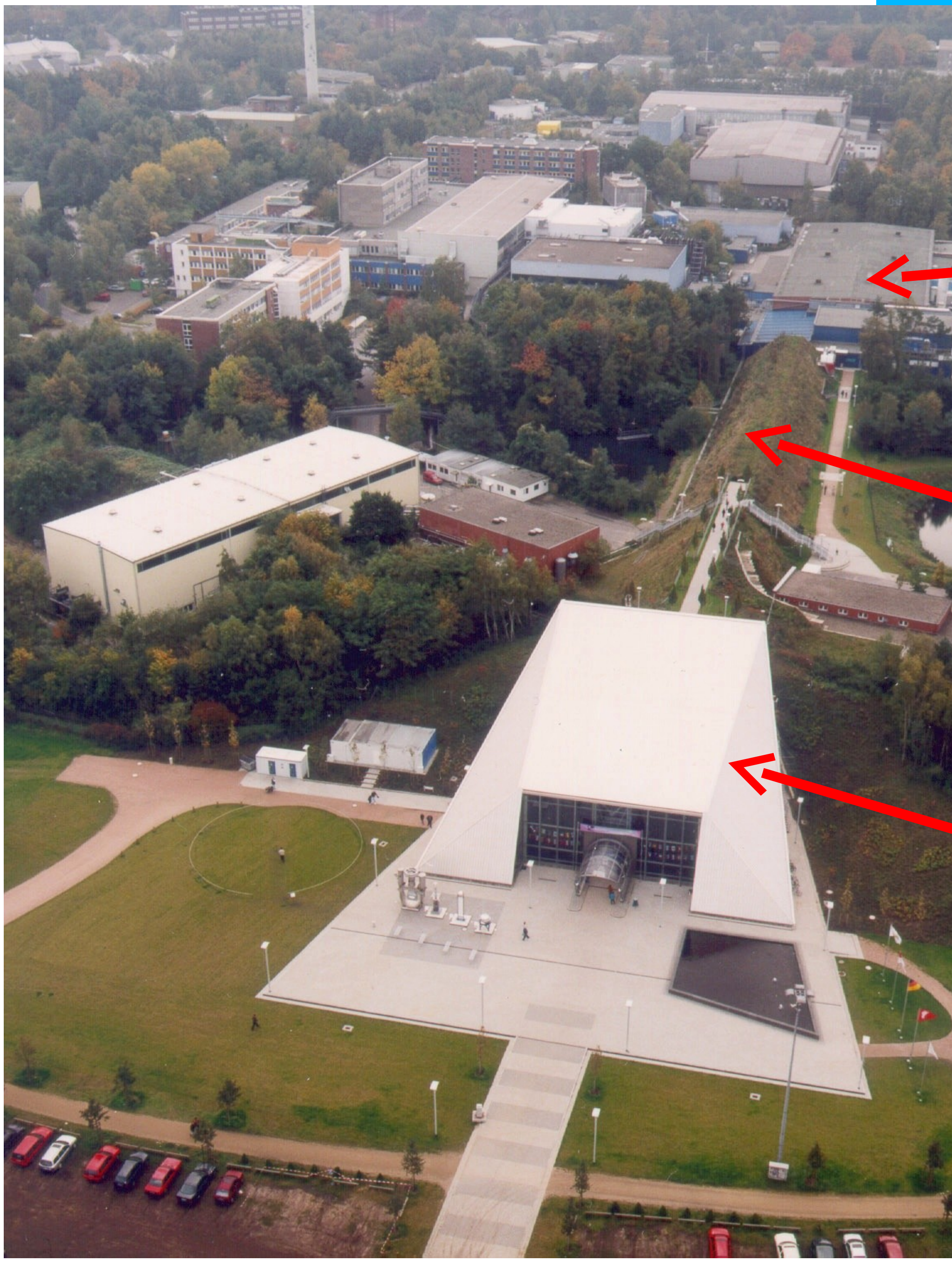
The general coupled Boltzmann equations for electron, $\rho^{(e)}(\mathbf{r},\mathbf{v},t)$, and ion densities, $\rho^{(i)}(\mathbf{r},\mathbf{v},t)$, where $i = 0, 1, \ldots, N_J$ denotes the ion charge, and $N_J$ is the maximal ion charge in the system are:

$$\partial_t \rho^{(e)}(\mathbf{r},\mathbf{v},t) + \mathbf{v}\cdot\partial_{\mathbf{r}}\rho^{(e)}(\mathbf{r},\mathbf{v},t) + \frac{e}{m}\left(\mathbf{E}(\mathbf{r},t) + \mathbf{v}\times\mathbf{B}(\mathbf{r},t)\right)\cdot\partial_{\mathbf{v}}\rho^{(e)}(\mathbf{r},\mathbf{v},t) = \Omega^{(e)}(\rho^{(e)},\rho^{(i)},\mathbf{r},\mathbf{v},t),$$

$$\partial_t \rho^{(i)}(\mathbf{r},\mathbf{v},t) + \mathbf{v}\cdot\partial_{\mathbf{r}}\rho^{(i)}(\mathbf{r},\mathbf{v},t) - \frac{ie}{M}\left(\mathbf{E}(\mathbf{r},t) + \mathbf{v}\times\mathbf{B}(\mathbf{r},t)\right)\cdot\partial_{\mathbf{v}}\rho^{(i)}(\mathbf{r},\mathbf{v},t) = \Omega^{(i)}(\rho^{(e)},\rho^{(i)},\mathbf{r},\mathbf{v},t).$$

These equations include the total electromagnetic force acting on ions and electrons. Collision terms, $\Omega^{(e,i)}$, describe the changes of the electron/ion densities of velocities $(\mathbf{v},\mathbf{v}+d\mathbf{v})$ measured at the positions $(\mathbf{r},\mathbf{r}+d\mathbf{r})$ with time. These changes are due to short-range processes, e. g. collisions, photoabsorptions. The number of processes involved in the sample dynamics depends on the radiation wavelength.

# FLASH FEL at DESY



Electron gun

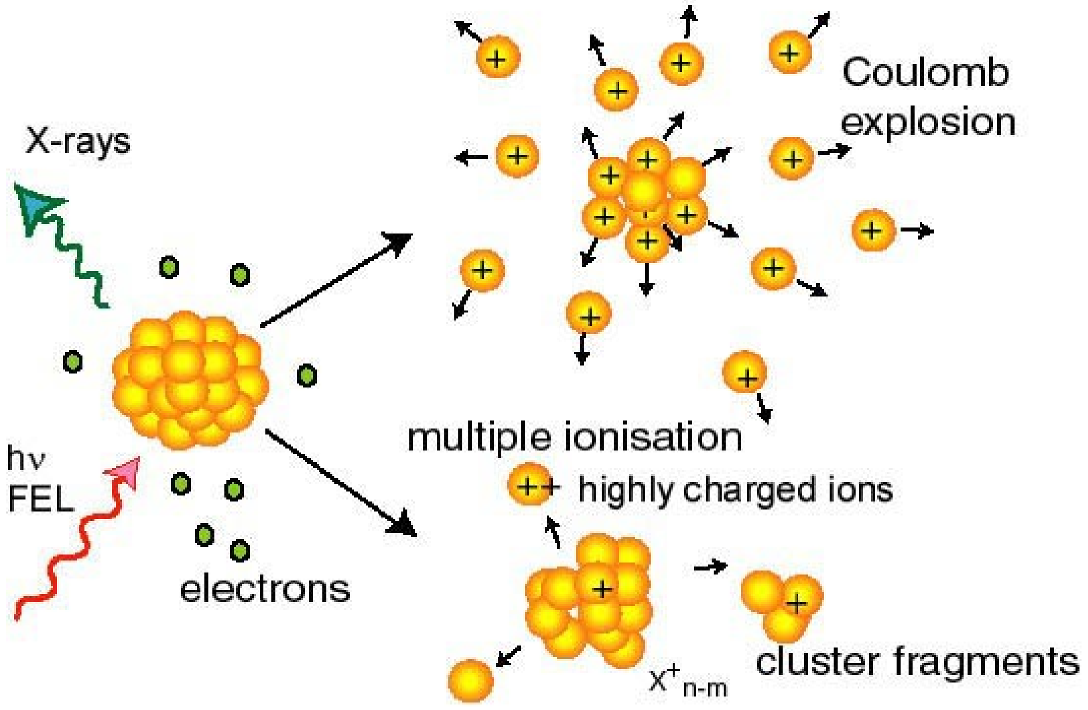
Linac and FEL undulator

Experimental hall (User Facility started July 2005)

**After upgrade:**
- 4,5- 50 nm
- 10-100 µJ
- 5 $GW_{peak}$
- 10-100 fs

DESY

# Experimental studies on clusters irradiated with intense FEL pulses




- **Mechanisms of energy absorption and ionization**
- **Non-linear / multi-photon processes observed?**
- **Timescales of electron emission and of ion motion**
- **New processes identified?**

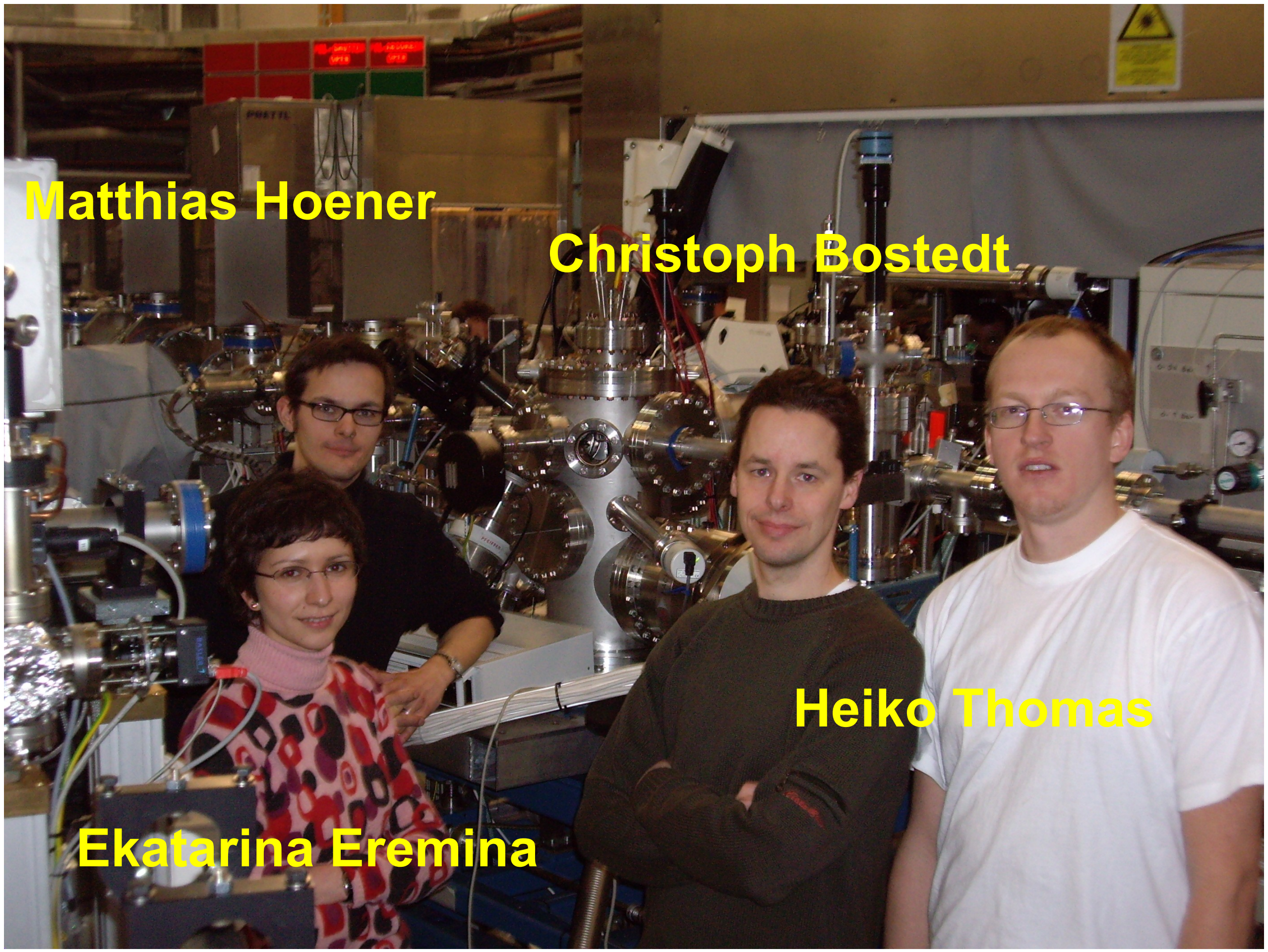
| | | |
|---|---|---|
| **λ= 100nm (2002)** | **32 nm/13 nm (2007-2009)** | **6 - 0.1 nm** |
| **valence electrons** | **valence/innershell electrons** | **atomic resolution** |

# Problems that have been studied ...

- Electron spectroscopy at 32 nm
- Evolution of heterogeneous clusters at 13/32 nm
- Imaging of atomic clusters at 13 nm
- Non-equilibrium evolution of irradiated liquid hydrogen at 13 nm

# The experimental group

Technische Universität Berlin




Thomas Möller

**Daniela Rupp**
**Markus Adolph**
**Lasse Landt**
**Sebastian Schorb**

**Collaboration:**
**H. Wabnitz[1], E. Ploenjes[1], M. Kuhlmann[1], E. Weckert [1], B. Ziaja[1]**
**Rubens de Castro[2],**
**Tim Laarmann[1],**
**K.H.Meiwes-Broer[4], J.Tiggesbäumker [4], T. Fennel [4]**
[1] DESY, [2] LNLS, Campinas Brasil, [4] Uni Rostock

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**R. Treusch, S. Düsterer, J. Feldhaus and the FLASH control room Team**

**Collaboration**
**with the groups of J. Hajdu ( Uppsala, Stanford) and H. Chapman (CFEL)**
**R. Hartmann, C. Reich, L. Strüder, MPG Halbleiterlabor**

# Evolution of irradiated samples

## Two phases:

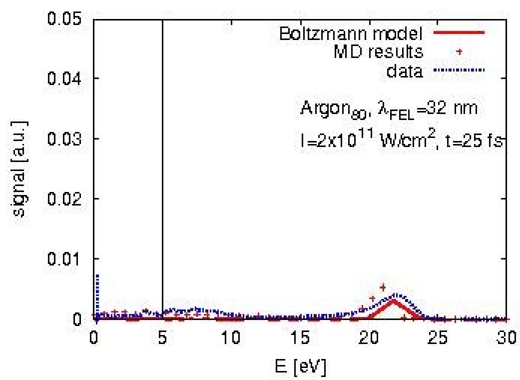
- non-equilibrium ionization phase: starts with the photon irradiation and lasts until thermalization of electrons and saturation of ionizations from ground state is reached

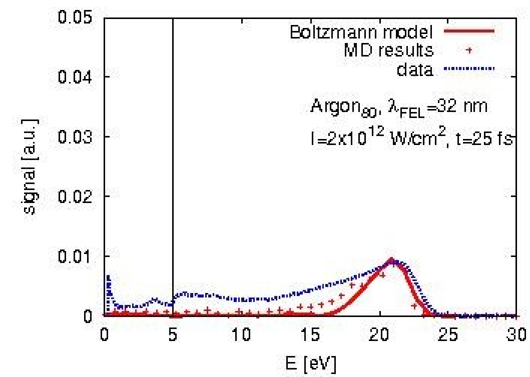
- semi-equilibrium expansion phase: electron-ion plasma in local thermal equilibrium, ions and electrons slowly escaping from outer shells → expansion of the sample

# Electron spectroscopy at 32 nm
# indication of energy absorption mechanisms

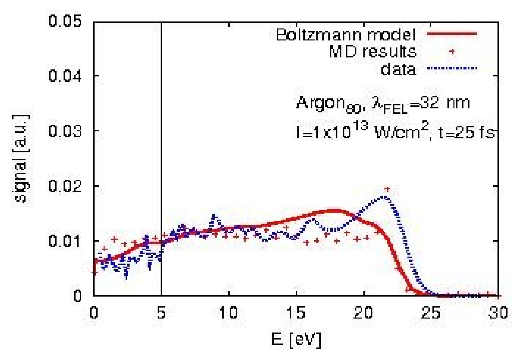
## Electron emission spectra at 32 nm for Ar(80) and Ar (150): sequential ionization

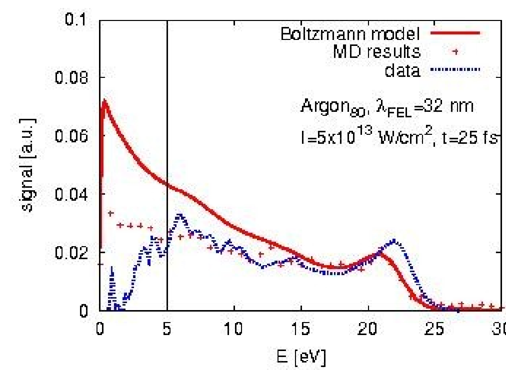
**[Ziaja et al., New J. Phys. 11 (2009) 103012]**




**FEL pulse length=25 fs**

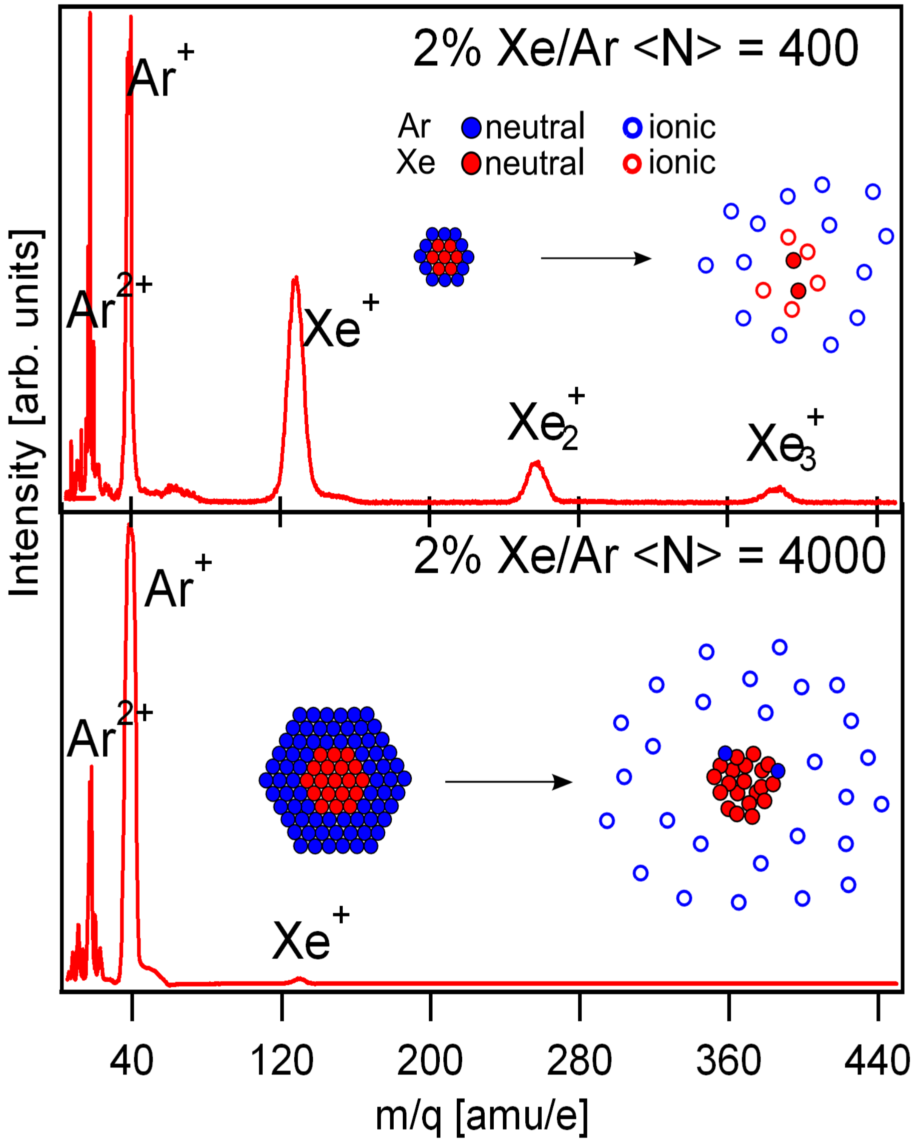



**Good agreement of the results with MD simulations by the Rostock group [T. Fennel et al.] and in-house MD simulations [F. Wang]**

DESY

# Coulomb explosion and delayed expansion in mixed Xe/Ar clusters at wavelength 13 nm ?




**13 nm/ 92 eV, $10^{14}$ W/cm$^2$**

**singly charged Ar ions from the surface**

**strong size effect**

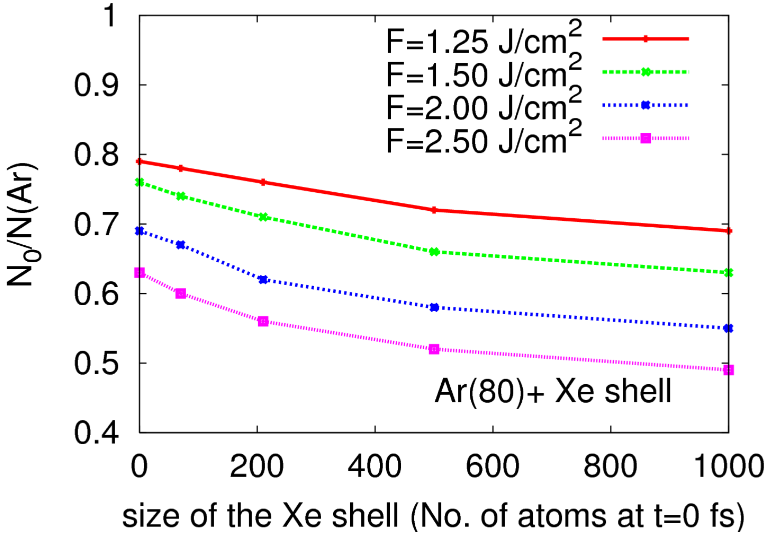
**Xe plasma in the interior recombines, neutral atoms?**

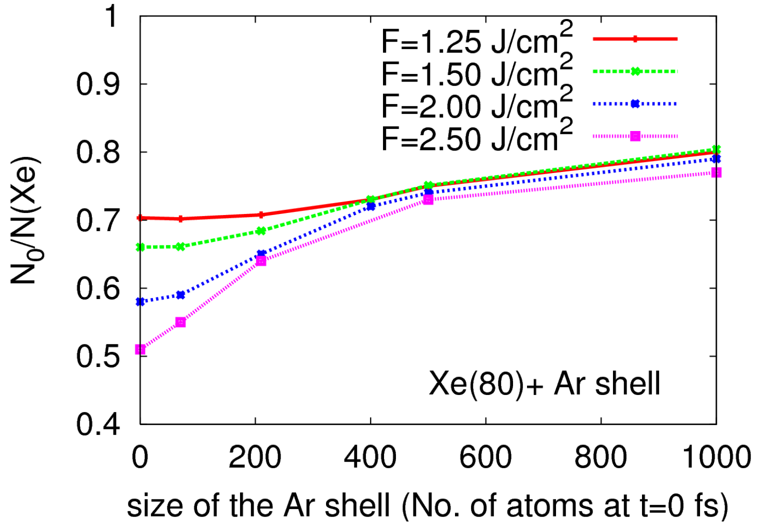
**delayed cluster expansion**

M. Hoener,et al J. Phys. B 41, 181001 (2008)

DESY

# Increased/decreased ionization in mixed Xe/Ar clusters at 32 nm: theory

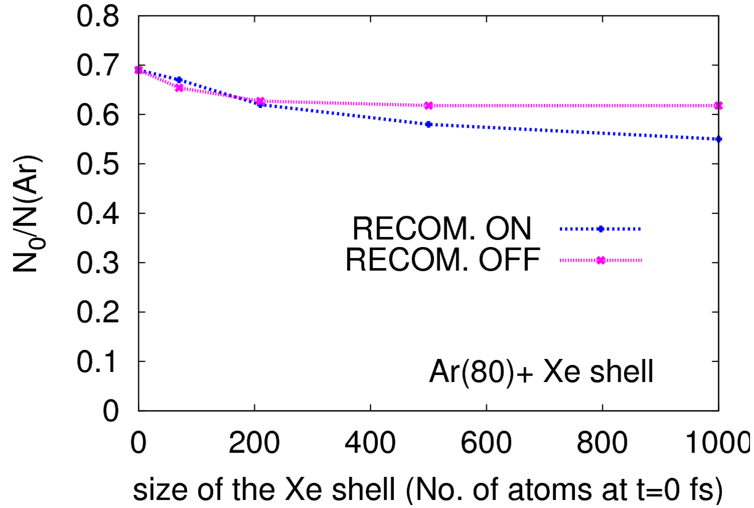


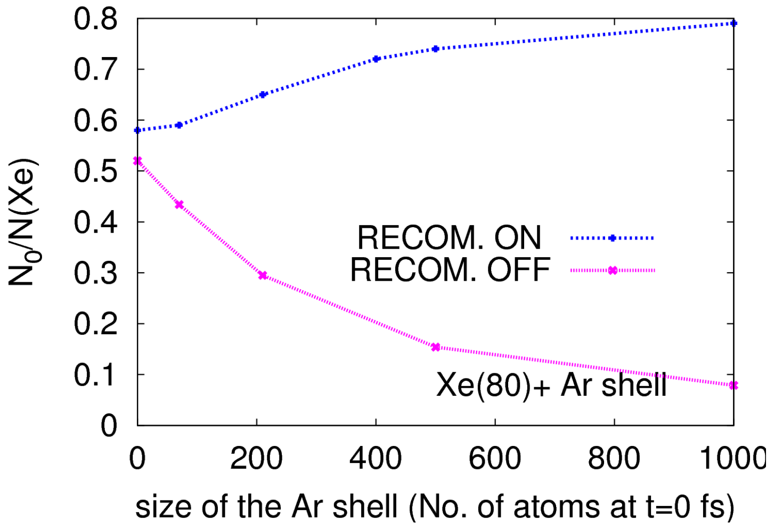




## 32 nm/ 40 eV, $10^{13}$ W/cm$^2$

- **Increased core ionization for Ar/Xe**
- **Decreased core ionization for Xe/Ar**

# Increased/decreased ionization in mixed Xe/Ar clusters at 32 nm: theory



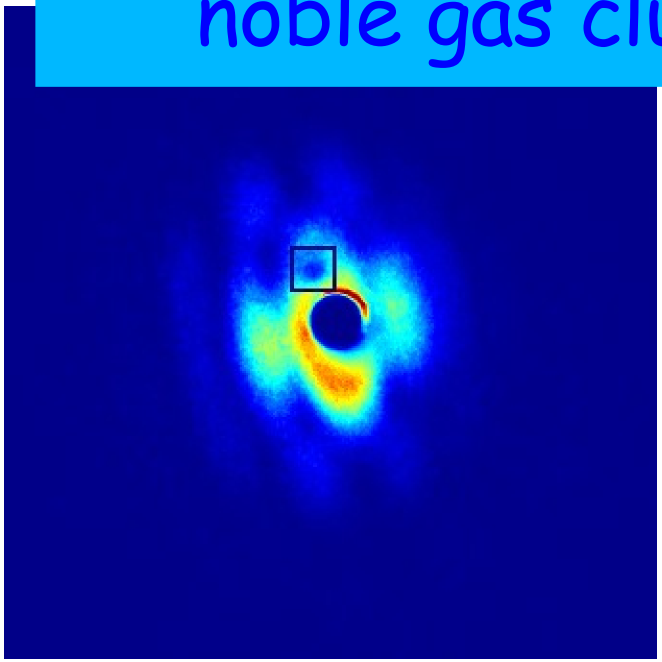




**Explanation: three-body recombination**

↓

**Consequences for single particle imaging**

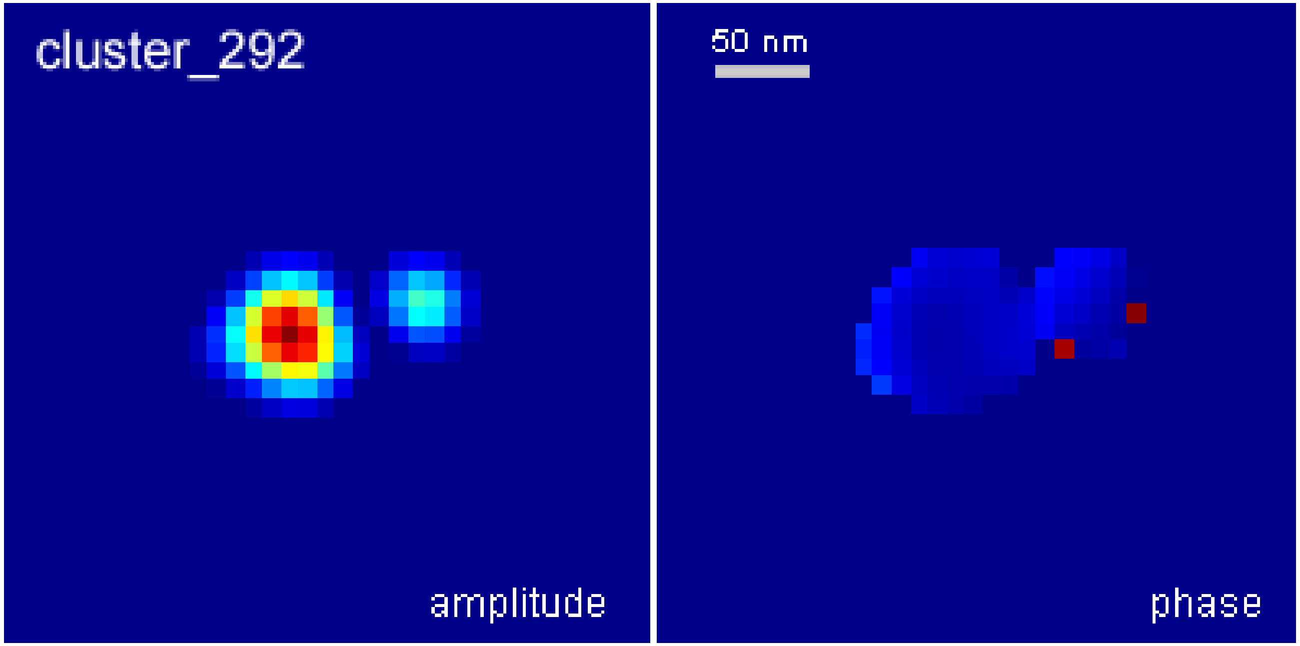
# Single shot scattering and imaging of large noble gas clusters at wavelength ~ 13 nm



[C. Bostedt, H. Chapman, F. Wang and T. Möller ]

scattering pattern

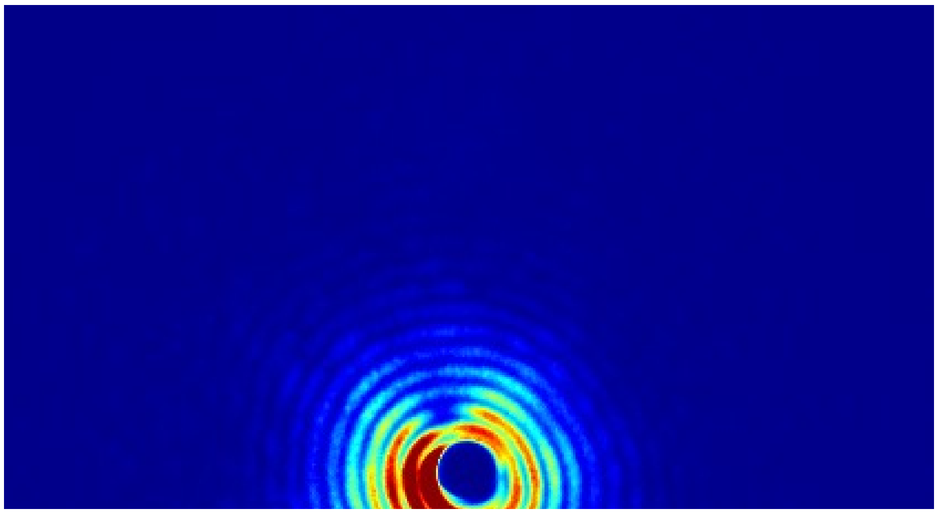
**Wavelength 13.7 nm**




reconstructed image

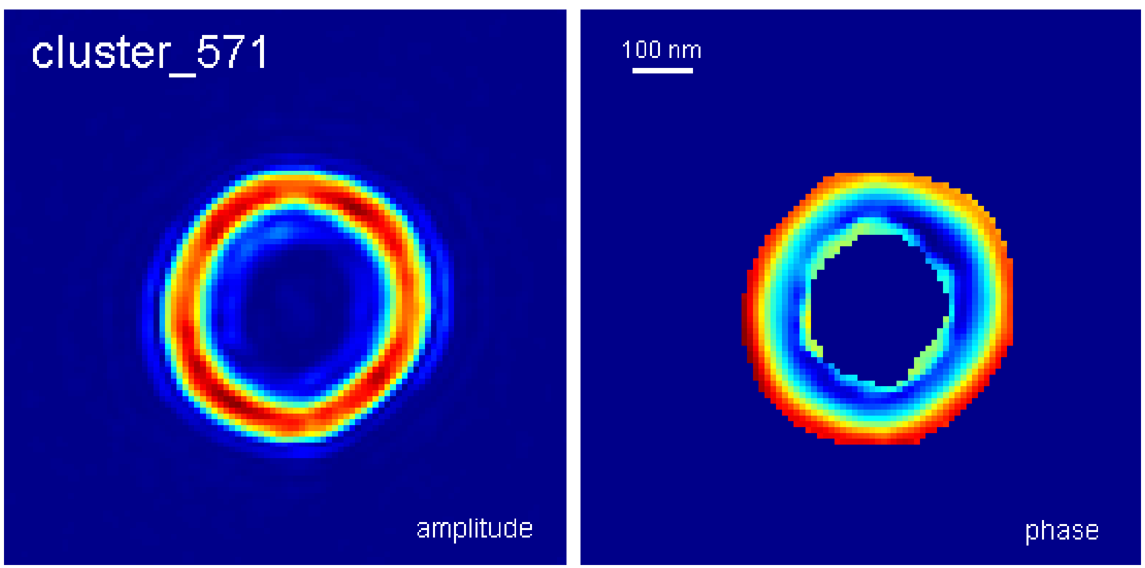
two clusters in direct contact

# Single shot scattering and imaging of large noble gas clusters at wavelength ~ 13 nm



scattering pattern

**Wavelength 13.7 nm**




reconstructed image

large cluster

penetration depth of light

# Soft X-Ray Thomson Scattering in Warm Dense Hydrogen

R.R. Fäustlin, S. Toleikis et al.

[Phys. Rev. Lett. 104 (2010), 125002]

# Collaboration

- **DESY, Hamburg**
  S. Düsterer, R.R. Fäustlin, T. Laarmann, H. Redlin,
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- **University of California, Berkeley**
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- **University of Jena**
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- **LLNL, Livermore**
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- **University of Oxford / RAL, Chilton, Didcot**
  G. Gregori, B. Li, J. Mithen, J. Wark
- **University of Rostock**
  T. Bornath, C. Fortmann, S. Göde, R. Irsig,
  K.-H. Meiwes-Broer, A. Przystawik, R. Redmer,
  H. Reinholz, G. Röpke, R. Thiele, J. Tiggesbäumker

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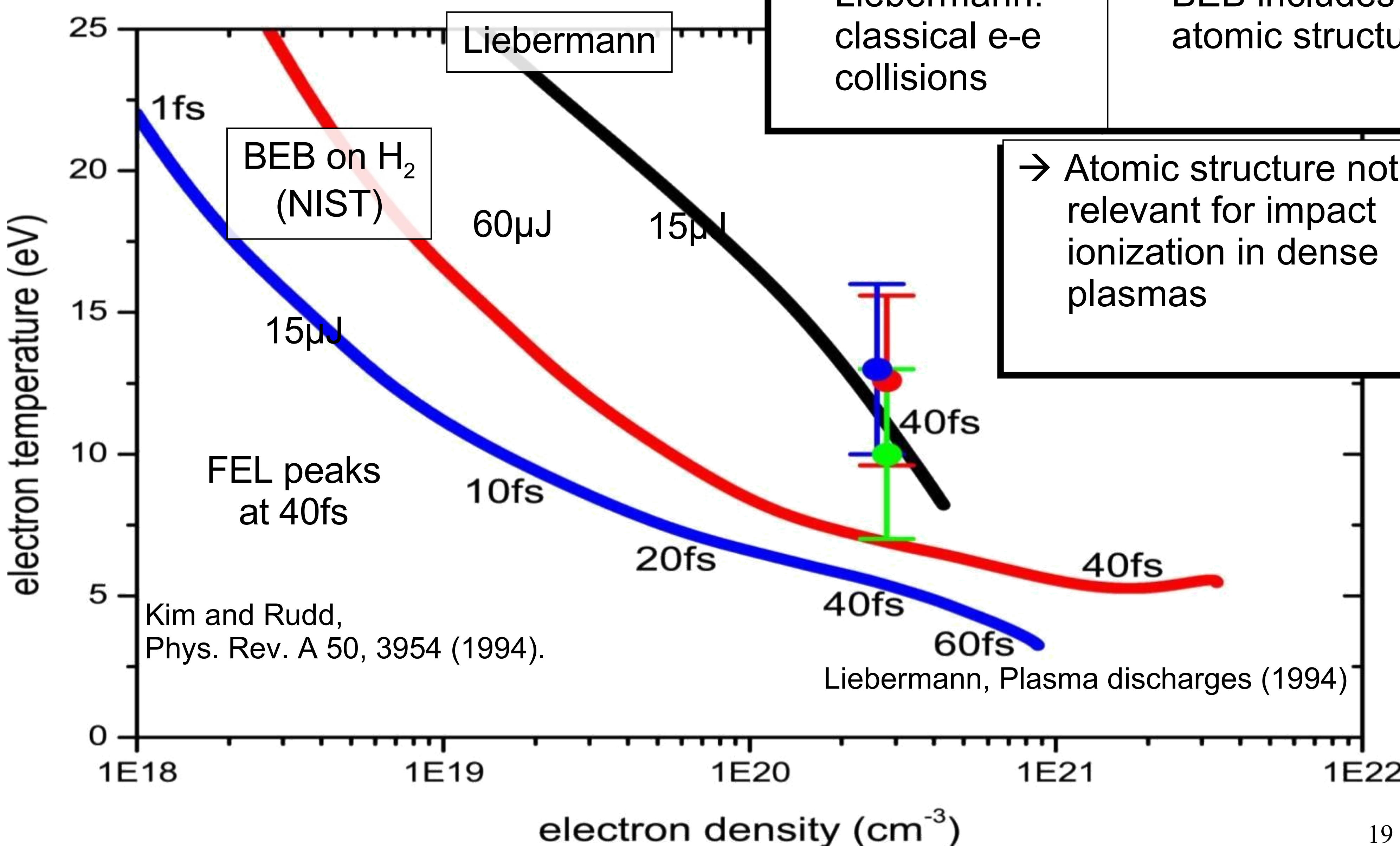
**European Community**: RII3-CT-2004-506008 (IA-SFS)

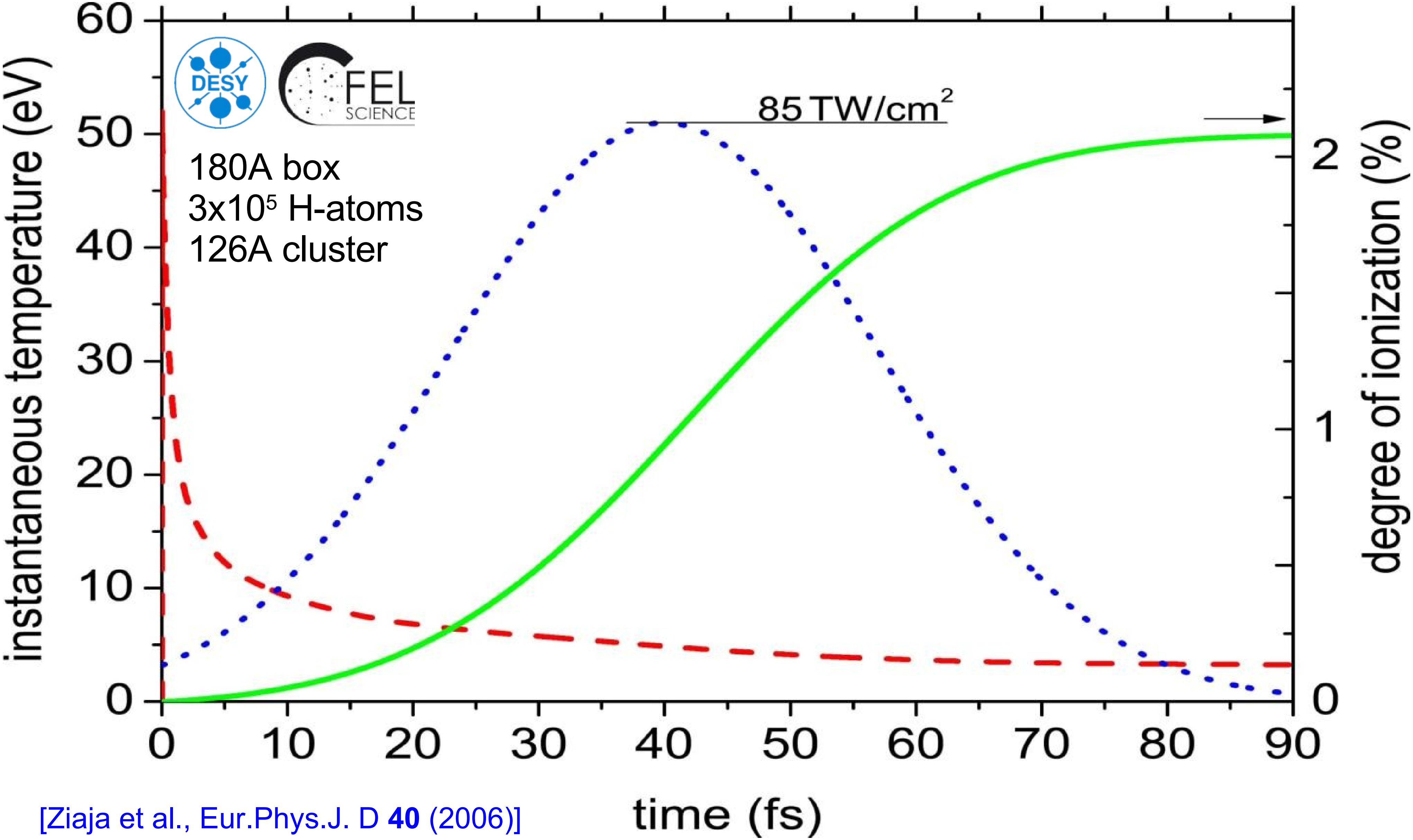
# We Validate Impact Ionization Models

- Liebermann: classical e-e collisions
- BEB includes atomic structure

→ Atomic structure not relevant for impact ionization in dense plasmas



# STS Probes fs Electron Thermalization




[Ziaja et al., Eur.Phys.J. D **40** (2006)]

# Summary and outlook

- **We constructed a useful tool for studying the evolution of FEL irradiated samples (computationally efficient treatment of large samples)**
- **Our model is so far the only one that gives an accurate description of all of the experimental data collected from atomic clusters at 100 nm and 32 nm wavelength**
- **Good agreement with data from warm dense matter hydrogen experiment at 13 nm**
- **Several problems can be studied in the next future:**
- **evolution of clusters irradiated with hard X-rays**
- **clusters of various structures**
- **mechanisms of slowing down the cluster explosion**
- **samples exposed to ultrashort FEL pulses**

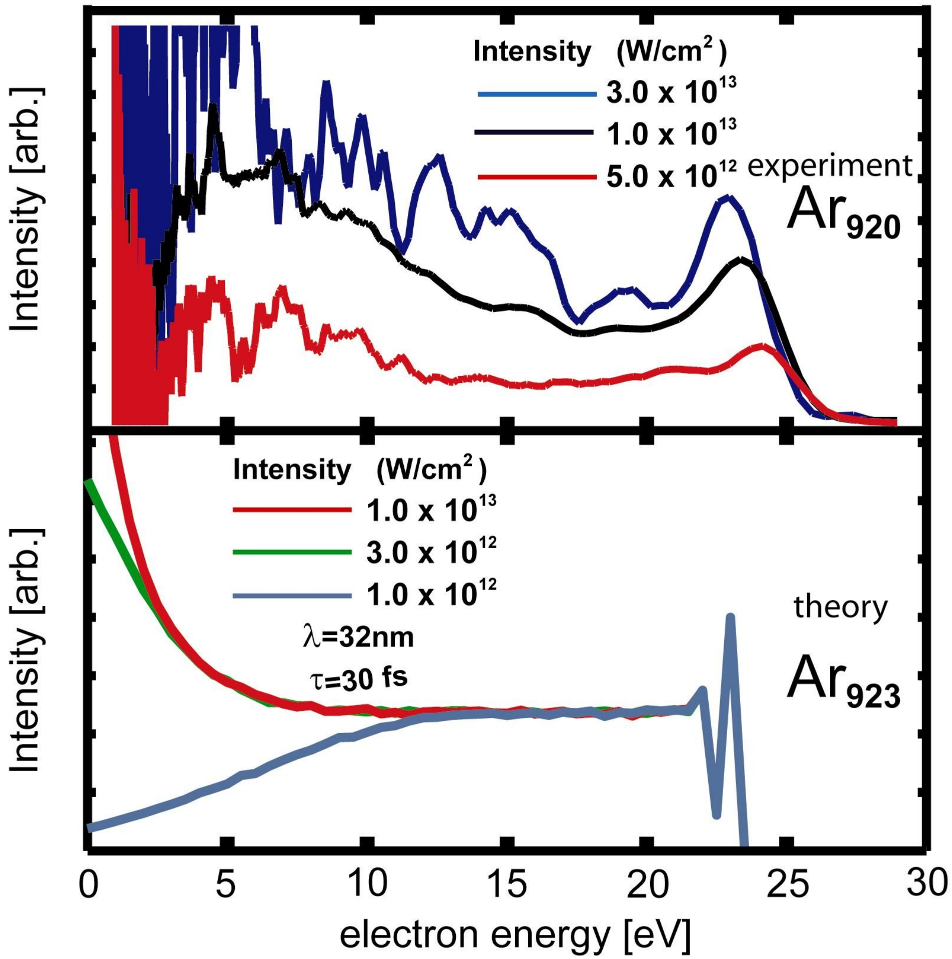
# Outlook: radiation damage by X-ray photons

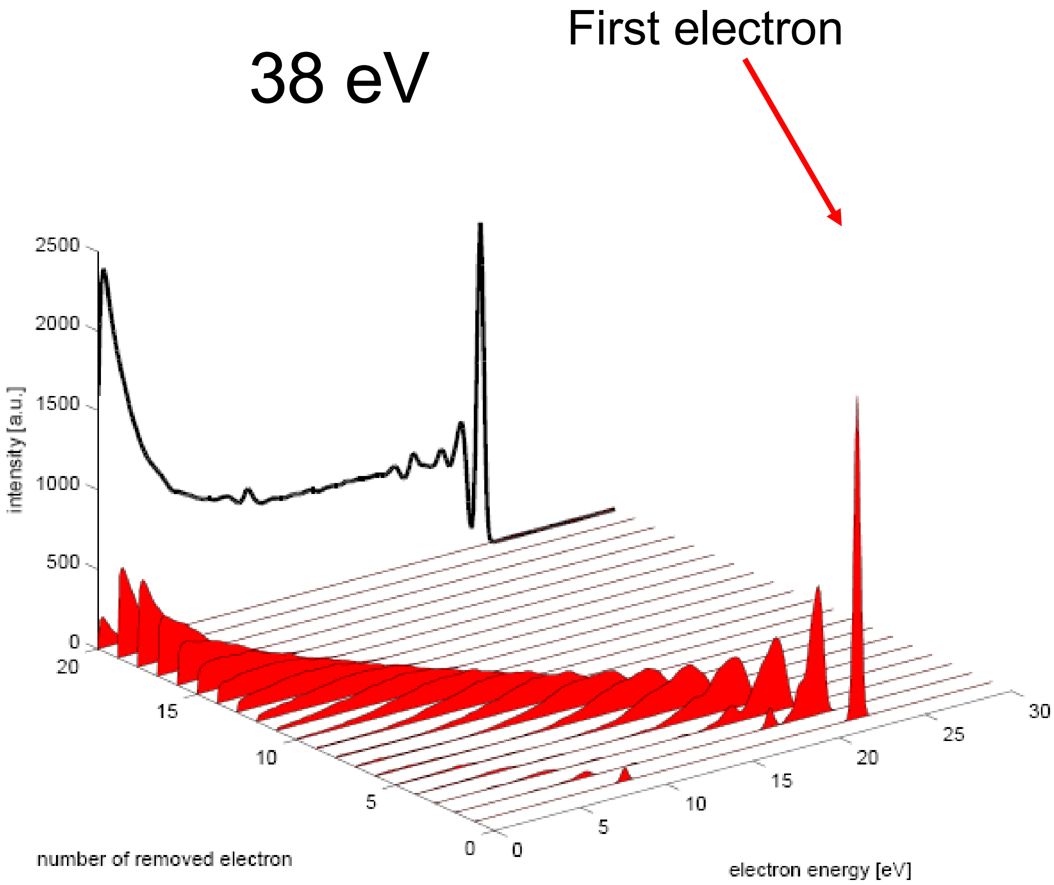
Basic processes contributing:

- photoionizations (from outer and inner shells) with subsequent Auger decays → inner-cascading within hollow-ions → many cascading paths for high Z elements
- collisional ionizations, elastic scatterings of electrons on atoms/ions
- long-range Coulomb interactions of charges with internal fields
- modification of atomic potentials by electron screening and ion environment
- recombination (3-body recombination)
- short range electron-electron interactions
- Compton scattering
- No inverse bremsstrahlung

**Boltzmann code is now being upgraded to hard X-ray regime!**

# Electron spectroscopy at 32 nm: indication of energy absorption mechanisms




**no thermionic electron emission**
**no plasma absorption [T. Fennel et al.]**

[C. Bostedt et al. Phys. Rev. Letters 100, 133401 (2008)]