XMDYN: Modeling radiation damage of XFEL irradiated samples

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Outline

- **Introduction** – modeling of matter at high x-ray intensities
- **XMDYN** – our approach
- **Applications**
  - – C60 @ LCLS
  - – Rare gas clusters @ SACLA

  } **Validation** of the model
  - – Single Molecule Imaging Start-To-End simulation (European XFEL)
- **Summary**

Introduction

Introduction

- **Hard X-ray Free-Electron Lasers**: ultrashort, intense pulses

E_{ph} ~ 0.5…10keV	T_{pulse} ~ 10...100fs	$N_{ph} \leq 10^{13}$	$I \leq 10^{21}$ W/cm^2

- Predominant process due to hard x-ray–matter interaction: **photoeffect**

  → highly ionized samples → **ultrafast dynamics** (sample damage)

- **Theoretical description** of the time evolution of the sample is needed

- **No \`ab initio\` approach** for large highly excited systems

  Models developed include

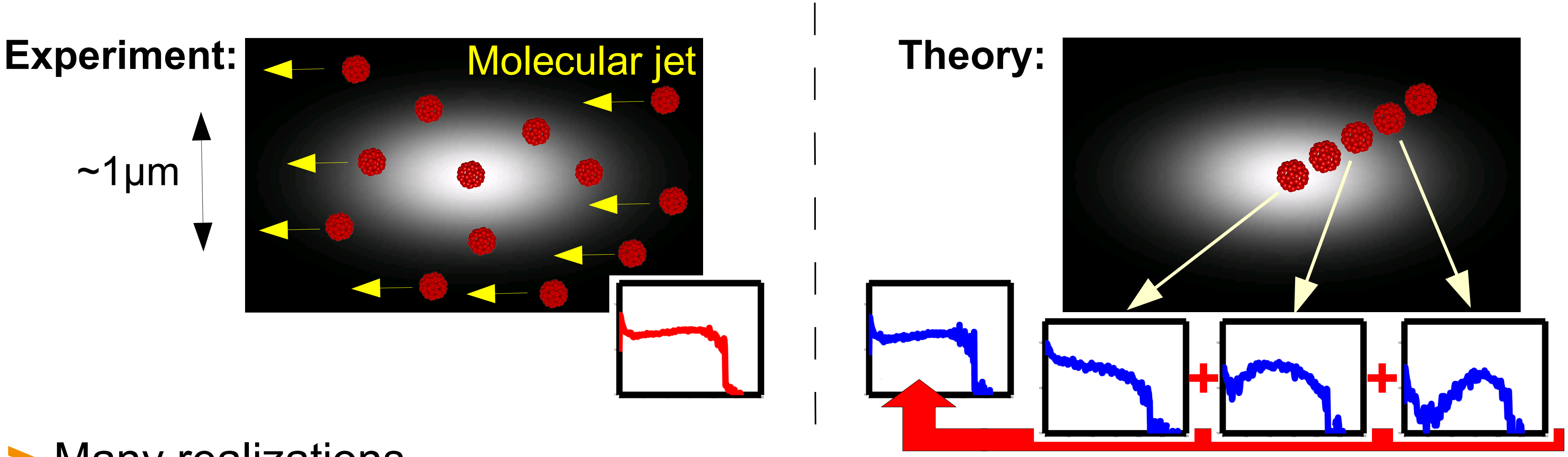
  – parameters from quantum calculations (rates, cross sections, ...)

  – classical physics (real space dynamics), simplifying assumptions

- Model **validation** is needed, e.g., via spectroscopy data

Modeling spectroscopy experiments – a challenge

- **Large number** of particles (atoms + electrons)
- System is **highly excited** (large number of ionizations)
- **Long** time (>ps) **propagation** (typical time-step ~as)
- Spatial intensity profile of the beam → **volume integrated signal**



- Many realizations

Experiment vs. Theory

XMDYN – our particle approach

Modeling with XMDYN

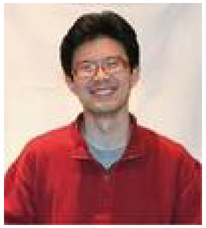
Atomistic Model + Molecular Dynamics (MD) in-house code

(core: Jurek, Faigel, Tegze, Eur. Phys. J. D **29**, 217 (2004))

- Bound electrons → **Occupation numbers**

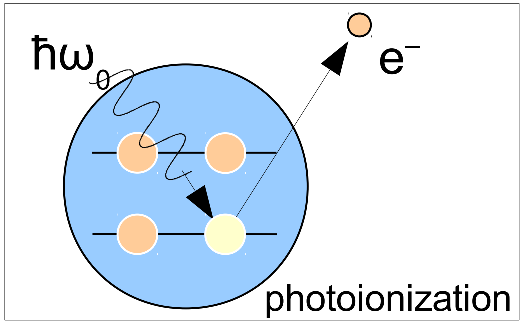
  Inner-shell processes (ph.eff./Auger/fluor.): Monte Carlo

  Rates by **XATOM** package (Sang-Kil Son, Robin Santra)




- **Real space dynamics**: MD
  - atoms/ions and (quasi-) free electrons: classical particles
  - classical force fields: Coulomb ; Newton's equations

- Phenomena due to the **molecular environment**
  - chemical bonds
  - secondary ionizations
  - molecular Auger effect



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XATOM – an integrated toolkit for x-ray and atomic physics

Sang-Kil Son, Robin Santra

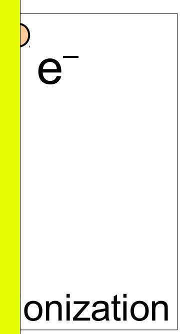
– **Ab initio calculated**

- photoionization cross section
- Auger and Coster-Kronig decay rate
- fluorescence rate
- elastic x-ray scattering cross section
- dispersion correction for elastic x-ray scattering cross section
- inelastic x-ray scattering cross section
- shake-off branching ratio
- effects of plasma environment

– **Ionization dynamics is described by rate equations**

– **Time-dependent populations obtained**

- charge state distribution
- pathways to reach high charge states
- scattering patterns including electronic radiation damage
- photoelectron / Auger electron / fluorescence spectra



Modeling with XMDYN

Atomistic Model + Molecular Dynamics (MD) in-house code

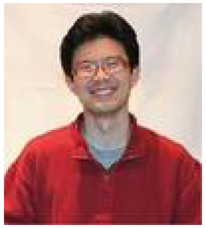
(core: Jurek, Faigel, Tegze, Eur. Phys. J. D **29**, 217 (2004))

- Bound electrons → **Occupation numbers**

  Inr … Carlo

  Parameters on-the-fly → heavy atoms

  Rates by **XATOM** package (Sang-Kil Son, Robin Santra)



- **Real space dynamics**: MD

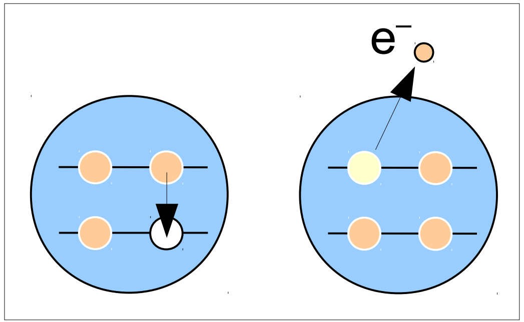
  – … s

  Efficiency: multi timestep ; GPU ; tree-code ;
  Hydrodynamic extension with XHYDRO code (V. Saxena)

- Phenomena due to the **molecular environment**

  XMOLECULE , XSOLID

  – molecular Auger effect



XMDYN – Applications

C_{60} @ LCLS

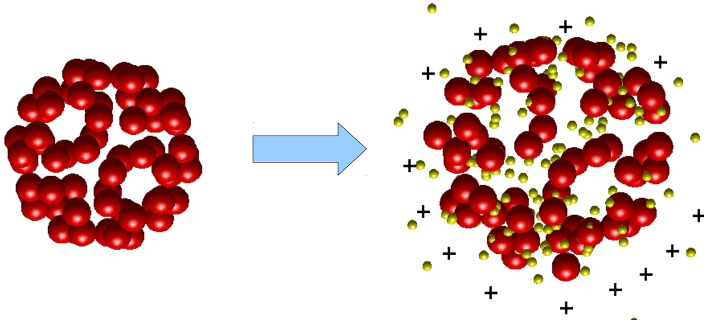
C_{60} @ LCLS – The Experiment

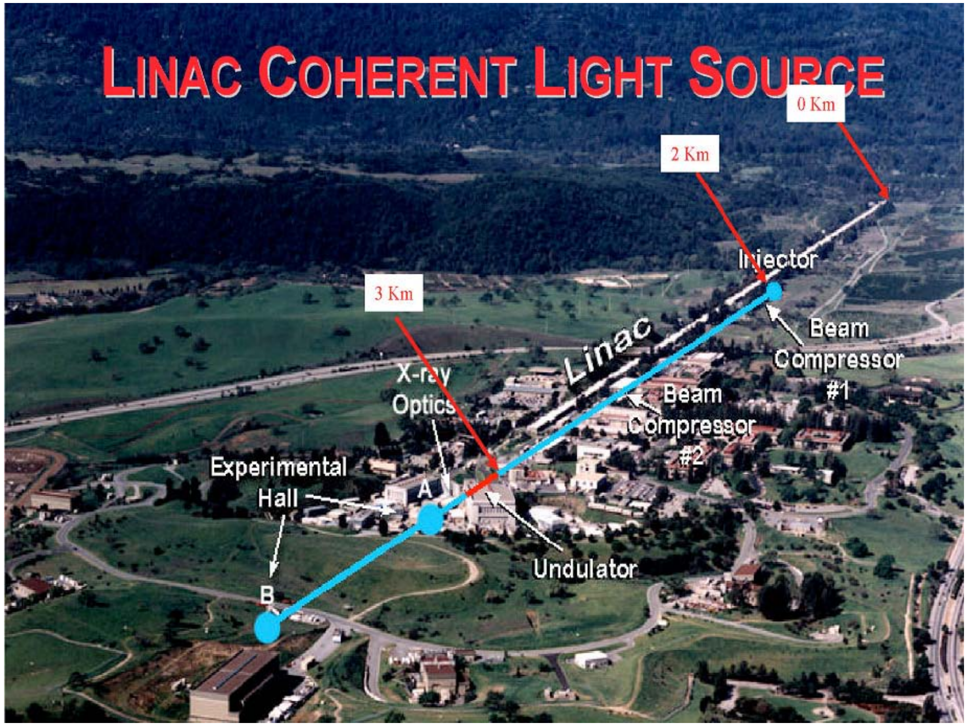
- **Nora Berrah** (WMU) *et al.*

  C_{60} molecules irradiated **at LCLS** (2012)

  E_{photon} = 485 / 600 / 800 eV

  T_{pulse} = 7 / 20 / 60 / 150 fs

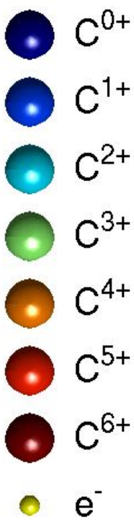


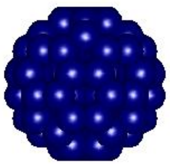


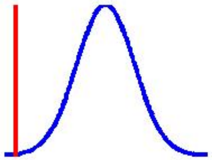
- Fragment M/Q distributions and energy spectra were measured

C_{60} @ LCLS – Strong ionization (high intensity) case

> Explosion in the focus







<u>Pulse parameters</u>:

T = 30fs,

E_{ph} = 485eV , ε = 0.345mJ,

focus = $(1.4\mu m)^2$

double Gaussian beam profile

Video: http://www.desy.de/infos__services/presse/pressemeldungen/2014/pm_270614/index_ger.html

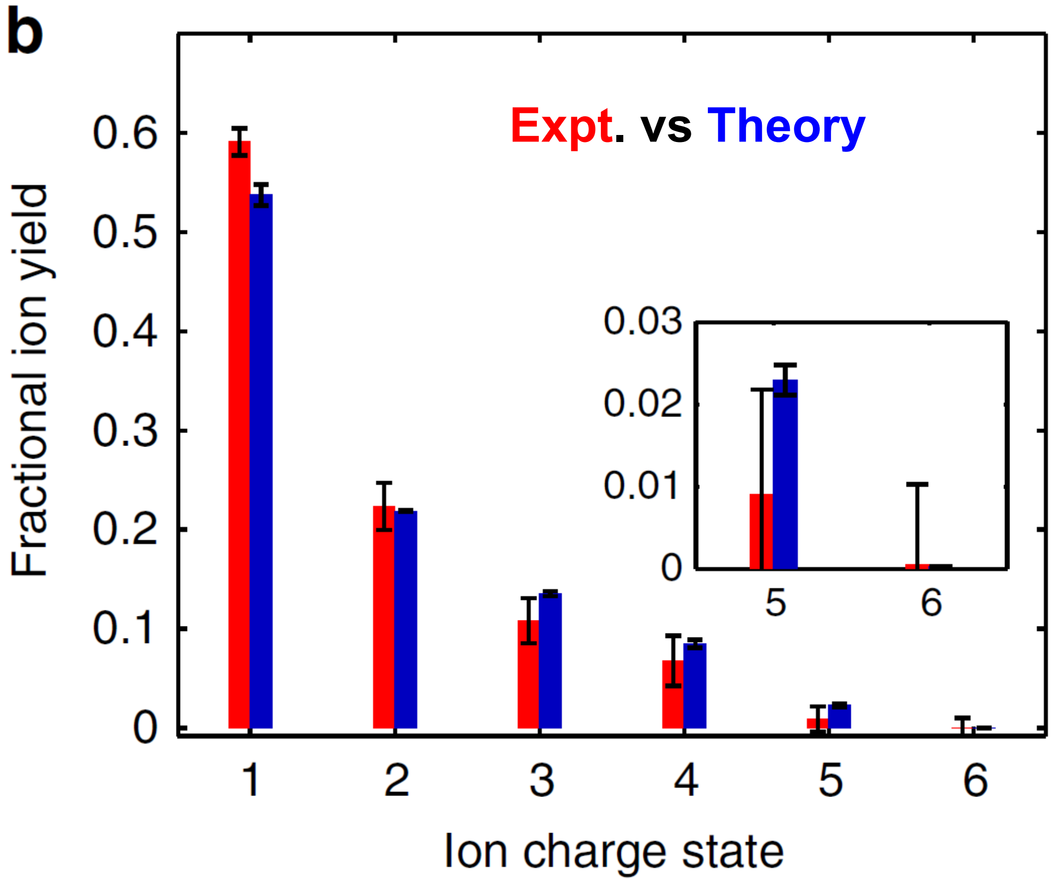
-40.0fs

B. Murphy *et al.*, Nat. Commun. **5** 4281 (2014)

C_{60} @ LCLS – Strong ionization (high intensity) case

> **Atomic ions** – experimental and volume integrated theoretical **yields**

Theory: **no parameter fitting**!



Pulse parameters:

Calibration based on Ar ion yields (XATOM, Sang-Kil Son)

T = 30fs ,

E_{ph} = 485eV, ε = 0.345mJ

focus = $(1.4\mu m)^2$

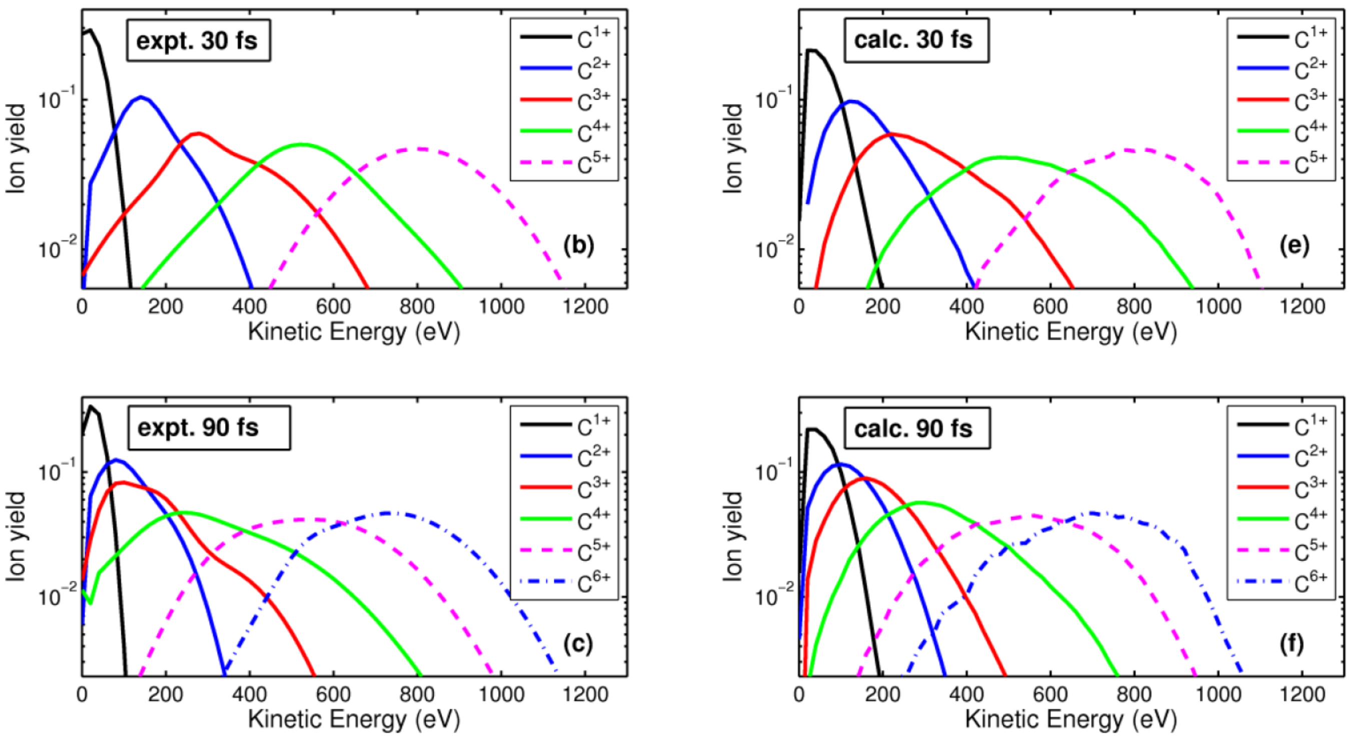
double Gaussian spatial profile

B. Murphy *et al.*, Nat. Commun. **5** 4281 (2014)

C_{60} @ LCLS – Strong ionization (high intensity) case

> Atomic ions – kinetic energy spectra

Theory: **no parameter fitting**!



Pulse parameters:

Calibration based on Ar ion yields (XATOM, Sang-Kil Son)

↓

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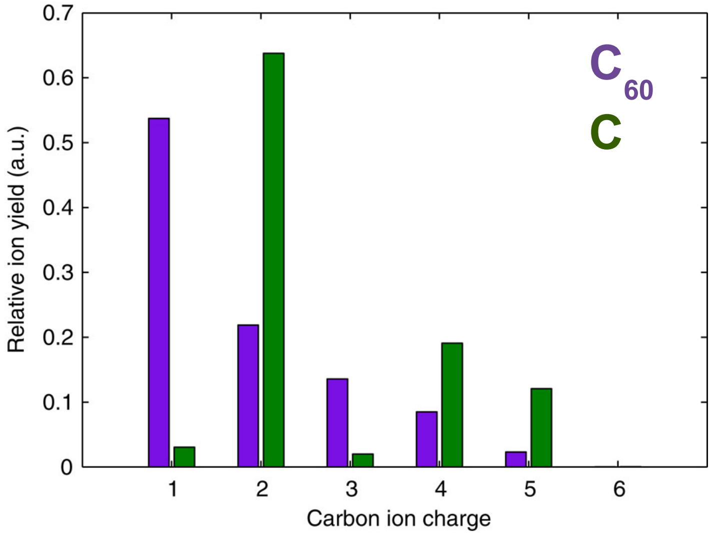
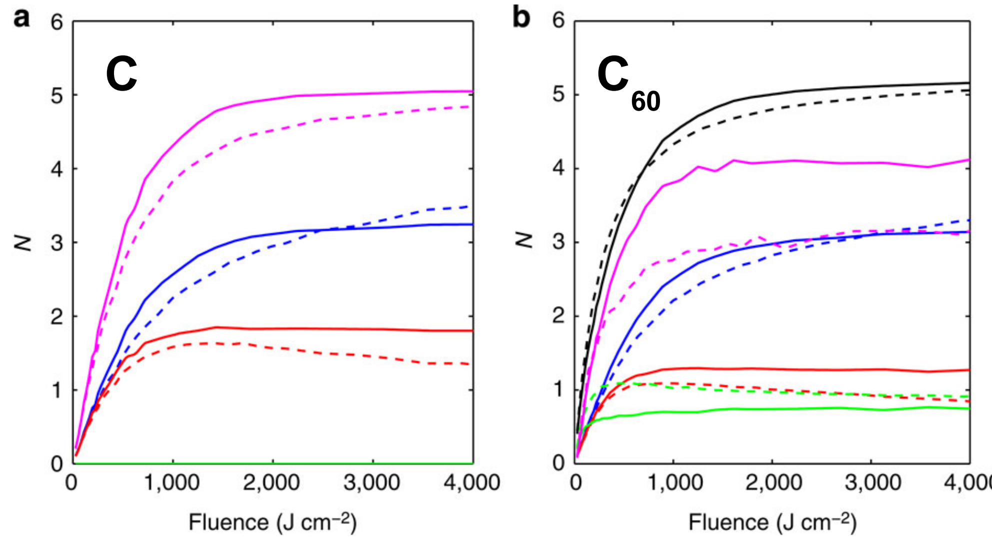
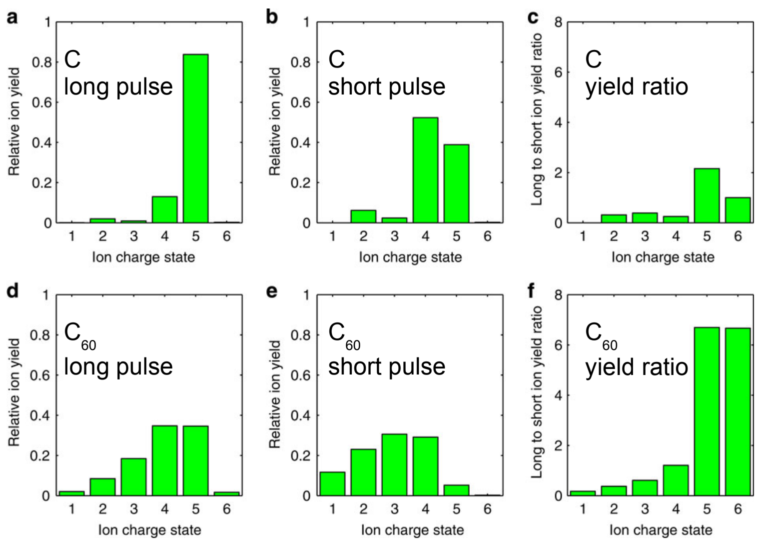
B. Murphy *et al.*, Nat. Commun. **5** 4281 (2014)

C_{60} @ LCLS – More physics







Long pulse
Short pulse

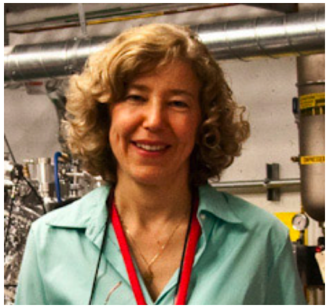
Number of events per atom:
photoionization
Auger decay
secondary ionizations
total ionization
Average final ion charge state

More details:

B. Murphy *et al.*,

Nat. Commun. **5** 4281 (2014)

C_{60} @ LCLS – The Collaboration



> Experiment: Nora Berrah

B. F. Murphy, T. Osipov, L. Fang, M. Mucke, J.H.D. Eland,
V. Zhaunerchyk, R. Feifel, L. Avaldi, P. Bolognesi, C. Bostedt,
J. D. Bozek, J. Grilj, M. Guehr, L. J. Frasinski, J. Glownia, D. T. Ha,
K. Hoffmann, E. Kukk, B. K. McFarland, C. Miron, E. Sistrunk,
R. J. Squibb, K. Ueda

> Theory: CFEL Theory Division

Z. Jurek, S.-K. Son, R. Santra

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XMDYN – Applications

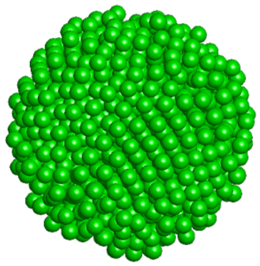
Rare gas clusters @ SACLA

Argon clusters @ SACLA – The Experiment

- **Kiyoshi Ueda** (Tohoku Univ.) *et al.*

  Ar, Xe clusters irradiated **at SACLA** (2012)

  E_{photon} = 5keV , T_{pulse} = 10fs



  size ~ 100 … 10000 atoms

- Electron kinetic energy spectra were measured

Argon clusters @ SACLA

- **Experiment: Kiyoshi Ueda**

  T. Tachibana, Z. Jurek, H. Fukuzawa, K. Motomura,

  K. Nagaya, S. Wada, P. Johnsson, M. Siano, S. Mondal, Y. Ito,

  M. Kimura, T. Sakai, K. Matsunami, H. Hayashita, J. Kajikawa, X.-J. Liu,

  E. Robert, C. Miron, R. Feifel, J. P. Marangos, K. Tono, Y. Inubushi,

  M. Yabashi, M. Yao

- **Theory: CFEL Theory Division**

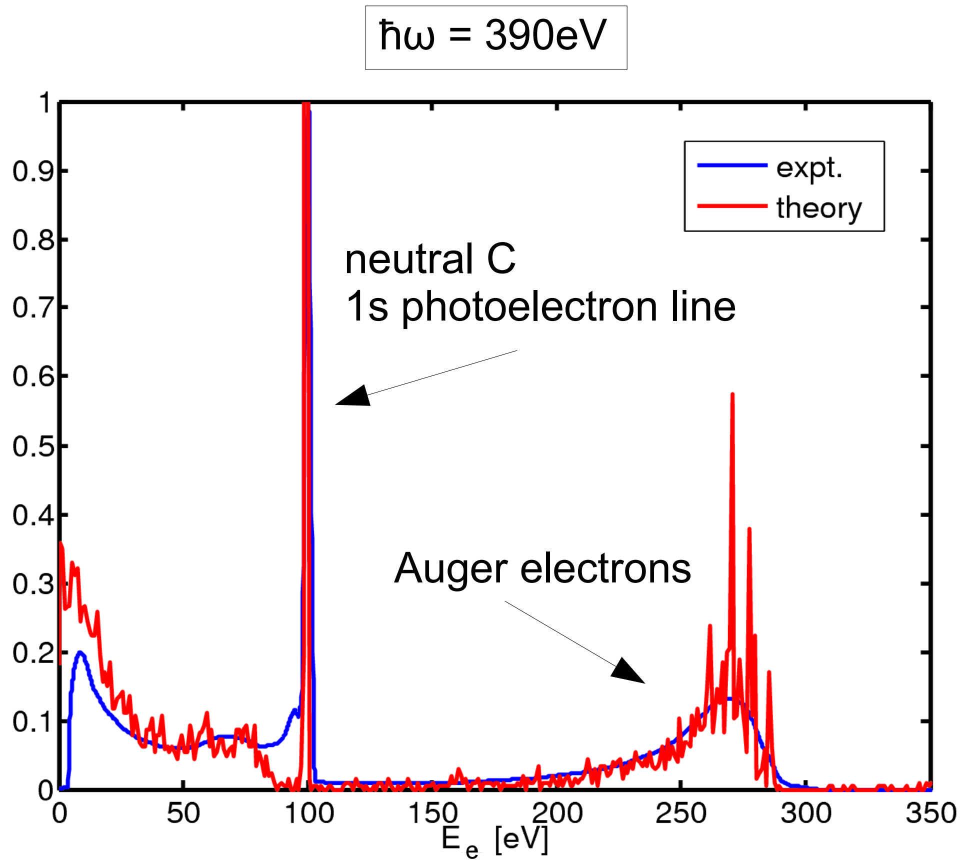
  Z. Jurek, S.-K. Son, B. Ziaja, R. Santra

XMDYN – Applications

Low intensity case: C_{60} @ synchrotron

Irradiated C_{60} – Low intensity (synchrotron) case

- Electron kinetic energy spectrum after single photoionization



– Experimental curve is from Hasylab report, 2003 (A. Reinköster, …, U. Becker)

– Theory:

no parameter fitting!

Z. Jurek, B. Ziaja, R. Santra, J. Phys. B **47** 124036 (2014)

XMDYN – Applications

Single Molecule Imaging Start-To-End (S2E)

Simulations

at the European XFEL

Single Molecule Imaging S2E Simulations – Collaboration

> Project Leader: Adrian P. Mancuso

Name	Organization	Role
Chun Hong Yoon	European XFEL & CFEL	Fast diffraction calculation, interfaces, much more
Liubov Samoylova	European XFEL	X-ray optics, propagation code
Alexey Buzmakov	Institute of Crystallography	Propagation code, interfaces
Oleg Chubar	Brookhaven National Lab	SRW Propagation code
Zoltan Jurek	CFEL	Photon–Matter Interaction Simulation
Sang-Kil Son	CFEL	Photon–Matter Interaction Simulation
Robin Santra	CFEL	Photon–Matter Interaction Simulation
Beata Ziaja	CFEL	Photon–Matter Interaction Simulation
Markus Kuster	European XFEL	Detector Effects
Julian Becker	DESY	Detector Effects
Heinz Graafsma	DESY	Detector Effects
Mikhail Yurkov	DESY	Source photon field simulations
Evgeny Schneidmiller	DESY	Source photon field simulations
Krzysztof Wrona	European XFEL	Scientific Computing, Image Reconstruction
Burkhard Heisen	European XFEL	Scientific Computing, Image Reconstruction
Duane Loh	NUS	Orientation Algorithms, Image Reconstruction
Andrew Aquila	European XFEL	X-ray optics, image reconstruction
Klaus Giewekemeyer	European XFEL	Scientific Computing, Image Reconstruction
Adrian Mancuso	European XFEL	Coordinator, Image Reconstruction
Thomas Tschentscher	European XFEL	European XFEL Director for optics and SPB

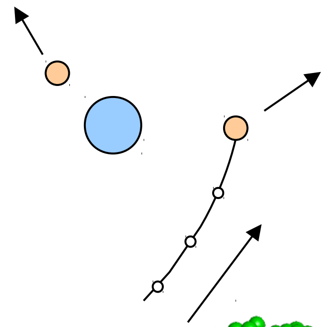
A. P. Mancuso, et al, Technical Design Report: Scientific Instrument Single Particles, Clusters, and Biomolecules (SPB), European XFEL (2013), doi:10.3204/XFEL.EU/TR-2013-004

CFEL SCIENCE

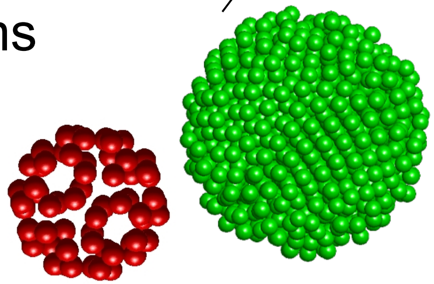
DESY

Summary

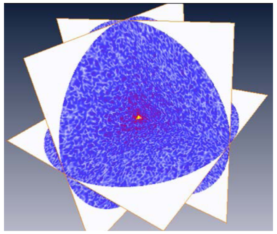
- **XMDYN**: modeling the dynamics of nanoparticles exposed to XFEL pulses.



- XMDYN applications: irradiated **rare gas cluster** systems and irradiated **C_{60}** molecules.



- XMDYN is used for **Single Molecule Imaging** studies, e.g. in the \`Start to End Simulation Project\` at the European XFEL.



- Further imaging and spectroscopy applications are planned and in progress

To be continued ...