Recent Science Highlights at Beamline 10.0.1 of the Advanced Light Source

Wednesday 24 Nov 2010 at 11:00 (01h00')

Beamline 10.0.1 of the ALS has typically a dozen or so of groups per year. These produce an average of 25 refereed papers and 4 articles of high impact (PRL, Nature or Science) per year. The beamtime is equally divided for groups doing condense matter physics and groups from the atomic and molecular community. A selected group of recent science highlights from the research done at this beamline will be presented.

Primary authors : Dr. AGUILAR, Alejandro (LBNL-ALS)

Co-authors :

Presenter : Dr. AGUILAR, Alejandro (LBNL-ALS)



Recent Science Highlights from Beamline 10.0.1 of the Advanced Light Source

Alex Aguilar Scientist Beamline 10.0.1

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Outline



- Beamline 10.0.1
- Condense Matter Physics
 - Angle Resolved Photoemission Spectroscopy (ARPES)
- Atomic and Molecular Physics
 - Velocity Map Imaging Spectroscopy
 - Photoelectron Spectroscopy (Scienta 2000) gas phase
 - Double Ionization Chamber
 - COLTRIMS
 - Photon-Ion Merged Beams Apparatus

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Photon-ion merged beams apparatus



 Photoionization of Se ions; Determination of elemental

abundances in PNe

Sterling et al., accepted JPB (2010)

N.C. Sterling, D. Esteves, A.L. Kilcoyne, E. Red, R.A. Phaneu R.C. Bilodeau, and A. Aguilar

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Section (Mb Determination of elemental

abundances in PNe

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Photoionization of Se ions;

 Photoionization of Ce@C₈₂⁺ Xe@C₆₀⁺; Confinement

resonances.

Quantum computing, Cancer therapy

Müller et al., PRL 101, 133001 (2008) Kilcoyne et al. PRL 105, 213001 (2010)

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Photon-ion merged beams apparatus



 $Se^+ + \gamma \otimes Se^{2+} + e^{-1}$

N.C. Sterling, D. Esteves, A.L. Kilcoyne, E. Red, R.A. Phaneu R.C. Bilodeau, and A. Aguilar



A. Müller, S. Schippers, M.Habibi, D. Esteves, J.C. Wang, R.A. Phaneuf, A.L.D. Kilcoyne, A. Aguilar and L. Dunsch



Photon-ion merged beams apparatus



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These experiments were only possible due to the high resolution and high photon flux of this beamline.

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Kilcoyne, E. Red, R.A. Phaneu R.C. Bilodeau, and A. Aguilar



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U10 Undulator



<u>U10 Undulator</u>

- 10.0 cm period, 43 periods
- 12 1500 eV energy range (@ 1.9 GeV)



www-xfel.spring8.or.jp/cband/j/Undulator.htm



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Beamline 10.0.1 Monochromator



Spherical Grating Monochromator

- 3 gratings: 380, 925, and 2100 lines/mm
- 17 340 eV energy range

Grating	Ruling (lines/	Energy Range
Low	380	17 - 75
Medium	925	40 - 170
High	2100	100 - 340



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Three Branch Lines (2 for AMO)





Angle Resolved Photoemission





Experimentally obtain E(k) dispersion & Fermi surface topology

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-0.8

the many-body

interaction from

spectral lineshapes

-0.4

E-E_p(eV)

Extract information on

0.0

Intensity (arb. units)

Two gaps in the cuprate superconductors





The pseudogap profile along the Fermi arc of La_{1.875}Ba_{0.125}CuO₄ reveals two distinct components.

This debunks a simple precursor scenario of pseudogap, and makes us rethink on the nature of pseudogap state.

Ruihua He et al. Nat. Phys. 5, 119 (2009)

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Iron pnictide superconductors

New type of high Tc superconductors other than cuprates

Wide range of photon energy, polarization control essential to study electronic structure $\Gamma \rightarrow \Gamma$

а Ē(s) 0.0 EB(eV) -0.2 -0.30.0 EB(eV) -0.1 -0.2 -0.3 0.0 EB(eV) -0.1 -0.2 -0.3 0.0 0.5 1.0 k_x (π/a)

Y. Xia et al. PRL 103, 037002 (2009) C. Liu et al. PRL 102, 167004 (2009) P. Vilmercati et al. PRB 79, 220503(R) (2009)

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Topological Insulators

Topology of electronic structure defines non-trivial metallic surface state

Spin can flow on the surface without backscattering

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Topological Insulators

First experimental realization of 3D topological insulator in Sn-doped Bi₂Te₃

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Mechanics of Photoionization

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- Incident photon energy ≥ ionization threshold
- A single electron is ejected without excitation

Photon

- BERKELEY LAB
- Incident photon energy ≥ ionization threshold
- A single electron is ejected without excitation

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- Excitation of an inner shell electron, followed by <u>autoionization</u>

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 Excitation of an inner shell electron, followed by <u>autoionization</u>

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 Excitation of an inner shell electron, followed by <u>autoionization</u>

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- BERKELEY LAB
- Excitation of an inner shell electron, followed by <u>autoionization</u>
- Lifetimes ≈ nanoseconds picoseconds

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- BERKELEY LAB
- Excitation of an inner shell electron, followed by <u>autoionization</u>
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- Excitation of an inner shell electron, followed by <u>autoionization</u>
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- BERKELEY LAB
- Excitation of an inner shell electron, followed by <u>autoionization</u>
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- BERKELEY LAB
- Excitation of an inner shell electron, followed by <u>autoionization</u>
- Lifetimes ≈ nanoseconds picoseconds
- Resonances occur at

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- BERKELEY LAB
- Excitation of an inner shell electron, followed by <u>autoionization</u>
- Lifetimes ≈ nanoseconds picoseconds
- Resonances occur at discrete energies

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Direct vs. Indirect Photoionization

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 As photon energy is increased, core electrons are excited to higher <u>discrete</u> energy levels

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etc.

'n =

n =

= 4/n = .3

- As photon energy is increased, core electrons are excited to higher <u>discrete</u> energy levels
- Higher principal quantum number, n

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etc.

 $= 4^{n} = .3$

- As photon energy is increased, core electrons are excited to higher <u>discrete</u> energy levels
- Higher principal quantum number, n
- Resonances follow selection real criteria

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= 4/n = 3

 $n = 5^{4}$

Indirect Ionization & Rydberg Series

18

Indirect Ionization & Rydberg Series

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Start with neutral sample

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Ionize the sample via electron/atom collisions in an Electron-Cyclotron-Resonance (ECR) Ion Source.

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Ionize the sample via electron/atom collisions in an Electron-Cyclotron-Resonance (ECR) Ion Source.

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Ionize the sample via electron/atom collisions in an Electron–Cyclotron–Resonance (ECR) Ion Source.

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Accelerate the Mixed Ions using a high voltage potential difference.

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Select the ion to be studied. The analyzing magnet selects based on the mass-to-charge ratio, magrence Berkeley National Laboratory

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Select the ion to be studied. The analyzing magnet selects based on the mass-to-charge ratio, magrence Berkeley National LABORATORY

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Merge the primary beam with a counterpropagating beam of photons using the merger_spherical_deflector_NAL LABORATORY

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Merge the primary beam with a counterpropagating beam of photons using the merger spherical deflector NAL LABORATORY

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Monitor the primary beam on the beam Faraday cup.

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Monitor the primary beam on the beam Faraday cup.

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Monitor the photon flux on a calibrated silicon photodiode.

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Determine the specific interaction region.

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Determine the specific interaction region.

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Count the photo-ions on a single particle channeltron detector.

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Simultaneously measure background using a mechanical photon chopper.

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Primary Ion

Se+

Beam





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<u>Photon Beam</u>

<u>Primary Ion</u> <u>Beam</u> Se+

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<u>Photon Beam</u>

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IPB Endstation





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IPB Endstation





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Experimental Results

Photoionization of Set

Motivations



- Se, Kr, and Xe ions have been observed in several planetary nebulae (PNe, ejected envelopes of low-mass stars).
- Due to their rarity (<= 10-9 the H abundance) only 1-2 ions of these elements are usually observed.
- Their relative abundances are good tracers of neutron-capture nucleosynthesis in evolved stars.





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• Model A

Included $4s^24p^2$, $4s4p^3$ and $4p^4$ configurations(3)

Gives rise to 20 levels from (3) configurations

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• Model A

Included 4s²4p², 4s4p³and 4p⁴ configurations(3) Gives rise to 20 levels from (3) configurations

• Model **B**

Included in addition several 3d-hole configurations 3d⁹4s²4p³; 3d⁹4s4p⁴; 3d⁹4p⁵ Gives rise to 126 levels from (6) configurations

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Included 4s²4p², 4s4p³and 4p⁴ configurations(3) Gives rise to 20 levels from (3) configurations

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• Model C

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Included 4s²4p², 4s4p³and 4p⁴ configurations(3)

Gives rise to 20 levels from (3) configurations

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Model C

Involved a 4d orbital instead of 3d-hole. Adding the configurations $4s^24p4d$, $4s^24d^2$, $4p^24d^2$, $4s4p^24d$ and $4p^34d$

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Involved a 4d orbital instead of 3d-hole. Adding the configurations $4s^24p4d$, $4s^24d^2$, $4p^24d^2$, $4s4p^24d$ and $4p^34d$

Gives rise to 246 levels from (8) configurations

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Se+ Photo-ion Spectroscopy

•27 scans

- •1 eV wide each
- Measured one-ata-time

 Can take several hours per-scan



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 Photon energy calibrated to Ar autoionizing resonances



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 Photon energy calibrated to Ar autoionizing resonances

 (side branch gas cell)



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 Photon energy calibrated to Ar autoionizing resonances

 (side branch gas cell)



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 Photon energy calibrated to Ar autoionizing resonances

 (side branch gas cell)

 7 absolute crosssection measurements



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 Photon energy calibrated to Ar autoionizing resonances

 (side branch gas cell)

 7 absolute crosssection measurements



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 Photon energy calibrated to Ar autoionizing resonances

 (side branch gas cell)

- 7 absolute crosssection measurements
- Complex resonant structure below the ⁴S ground



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Se+ High-Resolution Spectroscopy



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Se+ High-Resolution Spectroscopy



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Se+ High-Resolution Spectroscopy



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R. MexilenteworkshoptomAccelerMarks Physics: A Light Source





R. Mehienteworksheptemaccelenderks Physics: A Light Source





Physics: A Light Source

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 Measurements made at 2X & 3X the energy

• Nothing at 2X

 Matching features at 3X the energy (absolute at 54.56 eV)

 Corresponding features align



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Se+ Hi-Res Rydberg Series Analysisme

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Theoretical Analysis, Se⁺



Theoretical Analysis, Se+



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 The photon-ions merged beams method is the "cleanest" method (out of two) that allows highly accurate absolute photoionization cross section meassurements for single and multiply charge positive ions as well as negative ions.

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- These cross sections are needed in multiple disciplines and applications. For instance, EUV lithography light source modeling, Tokamak research, Astrophysics, FELs data, etc...

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- The photon-ions merged beams method is the "cleanest" method (out of two) that allows highly accurate absolute photoionization cross section meassurements for single and multiply charge positive ions as well as negative ions.
- These cross sections are needed in multiple disciplines and applications. For instance, EUV lithography light source modeling, Tokamak research, Astrophysics, FELs data, etc...
- Contrary to popular believe, in many cases (particularly heavy ions) these cross sections are not and can not be calculated yet, with sufficient accuracy for many of the applications. Therefore, these experiments are providing highly-accurate benchmarks for evolving

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- In the case of the absolute photoionization data for Se ions, the data helped on the...
 - 1. Clarification and determination of ionization thresholds
 - 2. Identify resonance features, including Rydberg series resonances
 - 3. Investigate parameters of beamline performance (pushing the beamline capabilities).

*see N.C. Sterling, et al, Pub.Astr. Soc. Australia, 26, 3, 339–344 (2009) LAWRENCE BERKELEY NATIONAL LABORATORY

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 - 1. Clarification and determination of ionization thresholds
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none of this would have been possible without a third generation light source.

*see N.C. Sterling, et al, Pub.Astr. Soc. Australia, **26**, 3, 339-344 (2009)

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Photon-ion merged beams apparatus



Photoionization of Se ions;

Determination of elemental

abundances in PNe

Sterling et al., accepted JPB (2010)

 Photoionization of Ce@C₈₂⁺ Xe@C₆₀⁺; Confinement

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Quantum computing, Cancer therapy

Müller et al., PRL 101, 133001 (2008) Kilcovne et al. PRI 105, 213001 (2010)

These experiments were only possible due to the high resolution and high photon flux of this beamline.

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Kilcoyne, E. Red, R.A. Phaneu R.C. Bilodeau, and A. Aguilar



A. Müller, S. Schippers, M.Habibi, D. Esteves, J.C. Wang, R.A. Phaneuf, A.L.D. Kilcoyne, A. Aguilar and L. Dunsch

Motivations



- From a single atom to a well structured solid sample.
- Attractive to have (manipulate) atoms isolated from their environment.
 - Building blocks for the qubits of quantum computers.
 - Chemical isolated reactive and poisonous atoms for medical imaging and cancer therapy.



Müller *et al.*, PRL 101, 133001 (2008)

Kilcoyne et al. PRL 105, 213001
While there are almost no experimental(20\$0)ts available for endohedral molecules in the gas phase, theoretical work flourishes without constraints. Clearly, experiments are needed to test and guide the theoretical developments

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Extremely difficult experiment "tour de France"







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Gracias por su atención



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Photoionization of endohedral fullerene ions Ce@C₈₂⁺ in comparison with atomic Ce^{q+} ions (q=2-4)

What is the charge of the atom inside the cage?



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EUV source candidates (13 -14 nm)





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Comparative Xe and Sn Spectra near 13.5 nm



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Photoionization of Low Charged Xe Ions





t = 400 nm

t = 600 nm

 Is photoionization of low-charged ions important for DPP and LPP source models?

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Photoionization of Low Charged Xe Ions





t = 400 nm

t = 600 nm



 Is photoionization of low-charged ions important for DPP and LPP source models?

- The blue lines indicate the 13.5 nm ± 2% (90.0 eV to 93.5 eV) region of interest for EUV lithography
- Strong absorption lines due to 4dnf autoionizing resonances are observed in both LPP and DPP.

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Alejandro Aguilar

Photoionization of Low Charged Xe Ions





Aguilar et al., "Absolute photoionization cross sections for Xe⁴⁺, Xe⁵⁺ and Xe⁶⁺ near 13.5 nm: Experiment and Theory", PRA 73 032717 (2006).

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Alejandro Aguilar