Gas phase/solid state Haxpes project at SOLEIL

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Outline

Introduction

RIXS and ultrafast nuclear motion (femtosecond Regime)

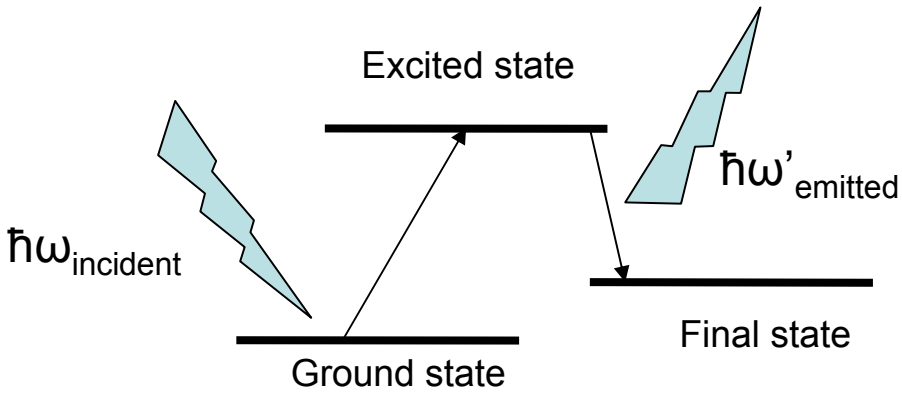
Scientific case in Atomic and Molecular Physics

Ultrafast nuclear motion (attosecond regime)
Recoil effect (vibrational and rotational)
Clusters

Design and schedule of the project

The GALAXIES beamline
Electron analyser

Resonant Inelastic X-Ray Scattering on Atoms and Molecules in the tender X-Ray region (2000eV-12 keV)



Resonant Raman regime, J.-Cl. Dousse (Fribourg, Switzerland); Phys. Rev. Lett. (2006)

RIXS on HCl: Subfemtosecond nuclear motion, M. Simon et al., Phys. Rev. A (2006)

Dispers./nondispers. at threshold, M. Zitnik (Ljubljana, Slovenia), Phys. Rev. A (2007)

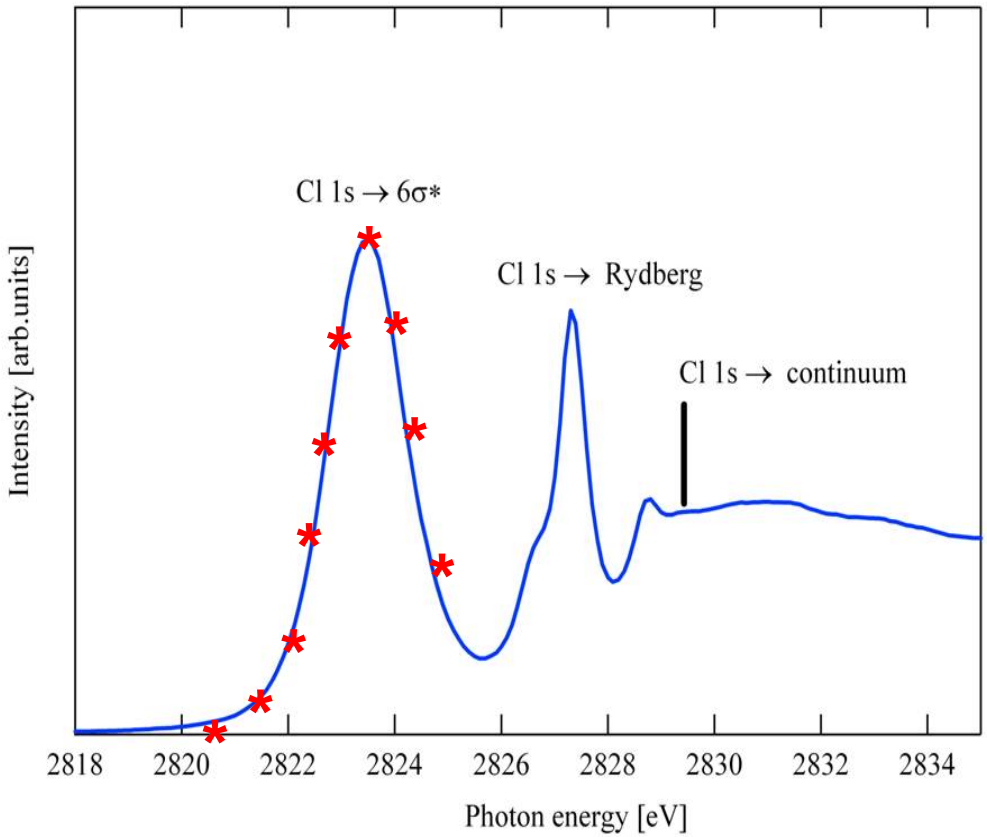
Polarisation measurements, D. Lindle (ALS, USA), Rev. Sci. Instrum. (2007)

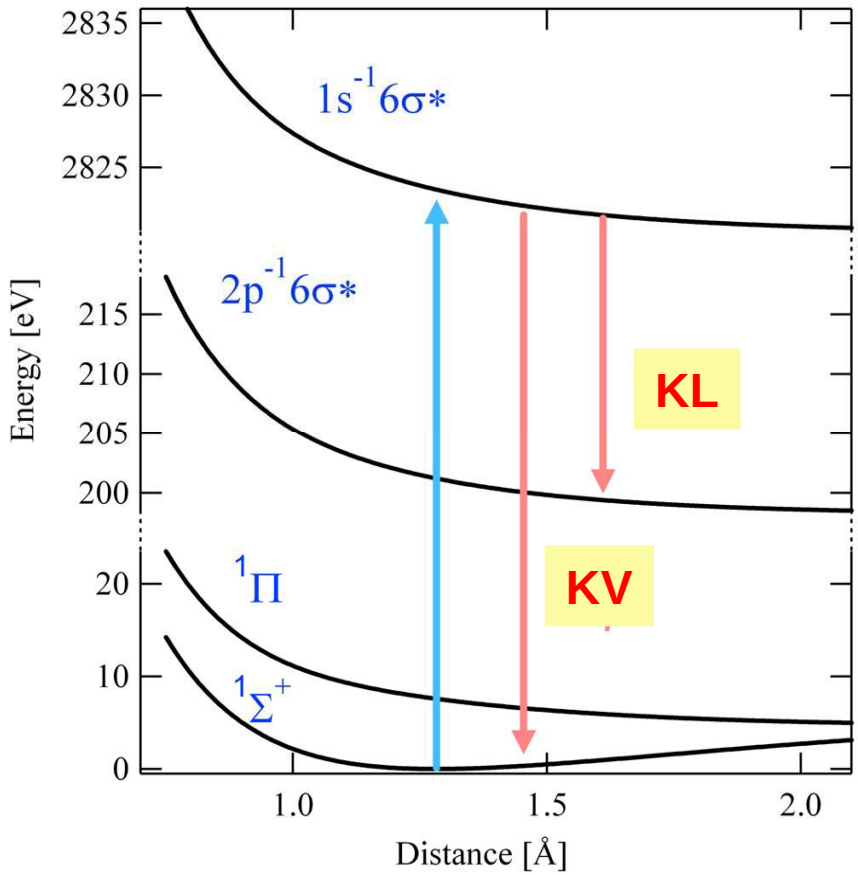
Linear dichroism in RIXS, R. Guillemin et al., Phys. Rev. Lett. (2008)

K shell Double Photoionization J.-Cl. Dousse et al., Phys. Rev. Lett. (2009)

Argon hypersatellites, M. Kavcic et al., Phys. Rev. Lett. (2009)

Ultrafast nuclear motion of K shell excited HCl molecule



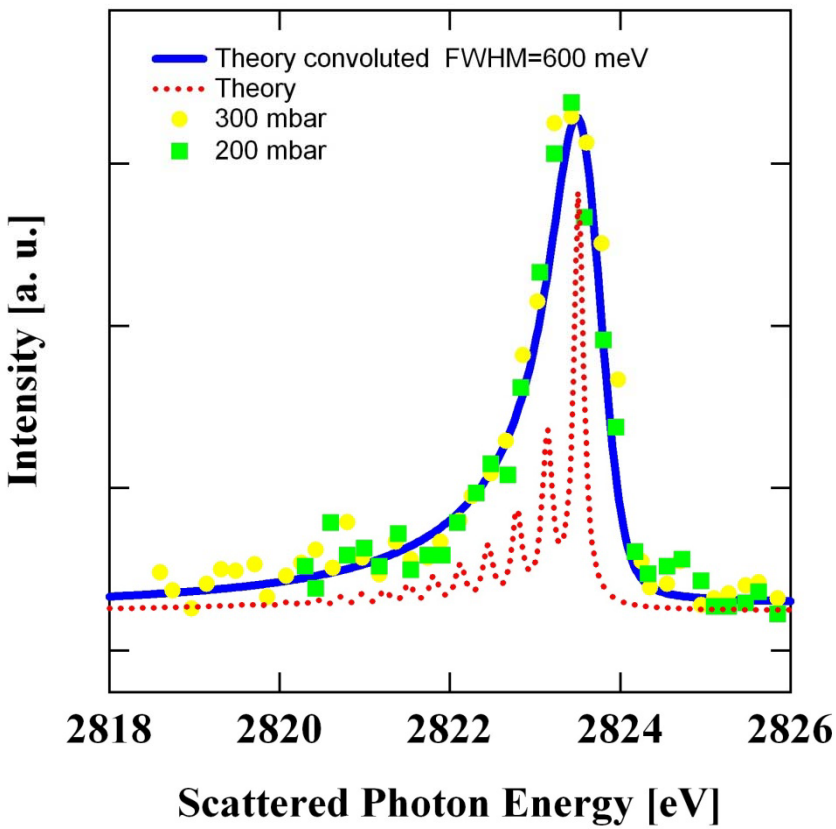


Absorption spectrum of gas-phase HCl around the Cl 1sthreshold.

Potential Energy Curves DFT

natural width τ

Elastic peak broadened by nuclear motion



Lifetime

1.05 femtosec

Chemical bond elongation: 10 picometers within 1 femtosecond

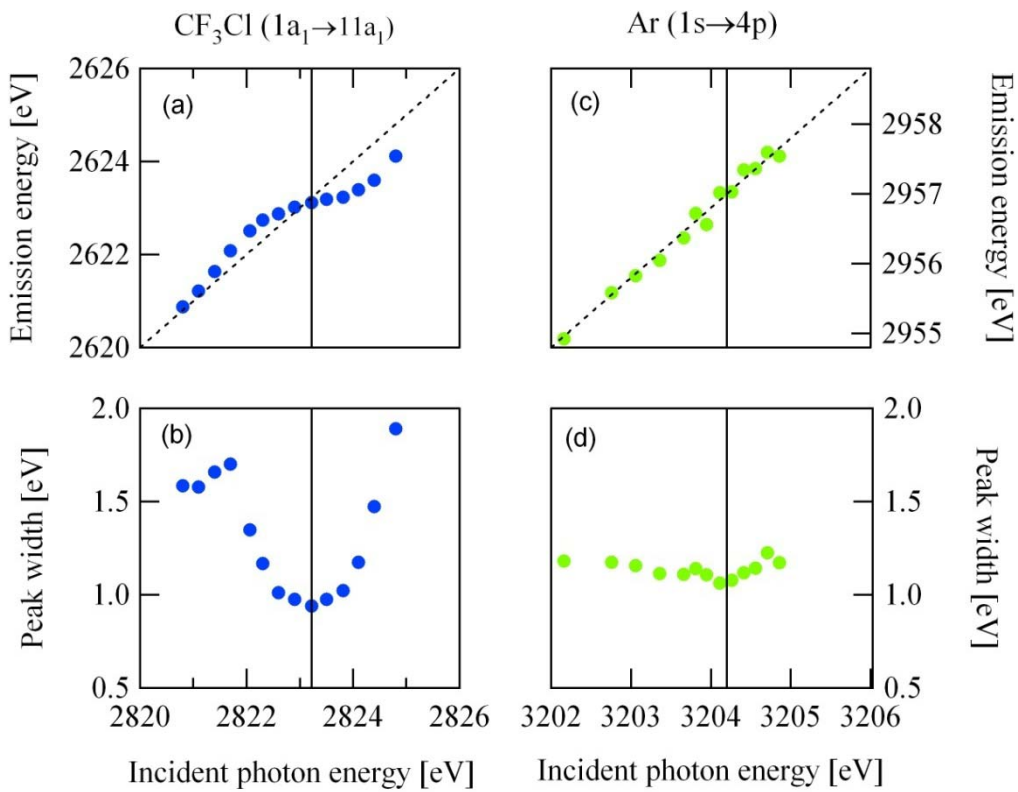
M. Simon, L. Journel, R. Guillemin, W. C. Stolte, I. Minkov, F. Gel'mukhanov, P. Salek, H. Ågren, S. Carniato, R. Taïeb, A. C. Hudson, and D. W. Lindle, **Phys. Rev. A** 73 (2006) 020706

Molecular features in RIXS

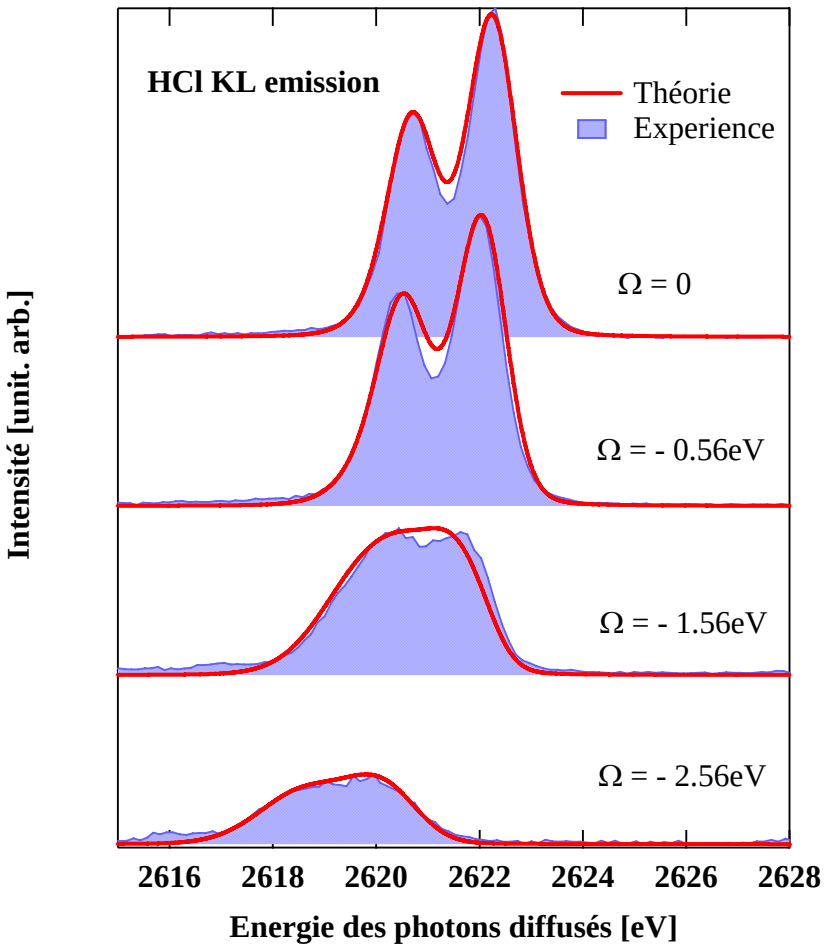
Comparison with atomic RIXS

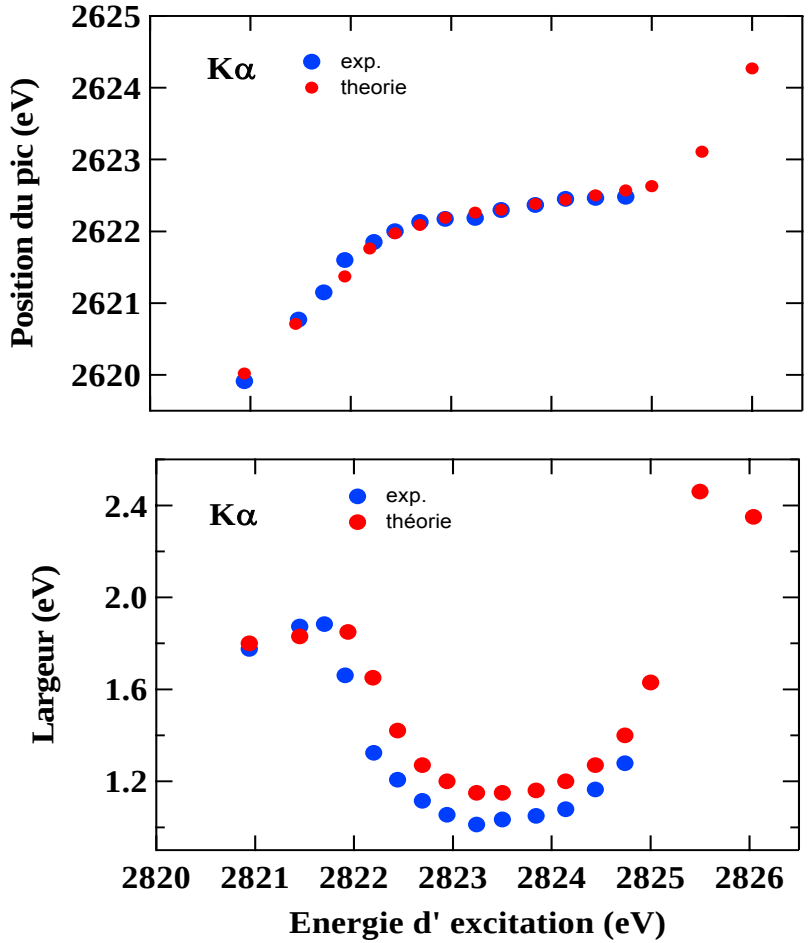
General conclusion: RIXS in molecules driven by the topology of PES of the initial, intermediate, and final states.

Nuclear dynamics of the core-excited state.



Resonant Kα emission of the HCl molecule





2 spin-orbit component: $2p_{3/2}$ and $2p_{1/2}$

Width and dispersion depend on the energy detuning Ω.

M. Simon et al. Phys. Rev. A 73, 020706 (2006)

HAXPES: Gas phase and Solid state

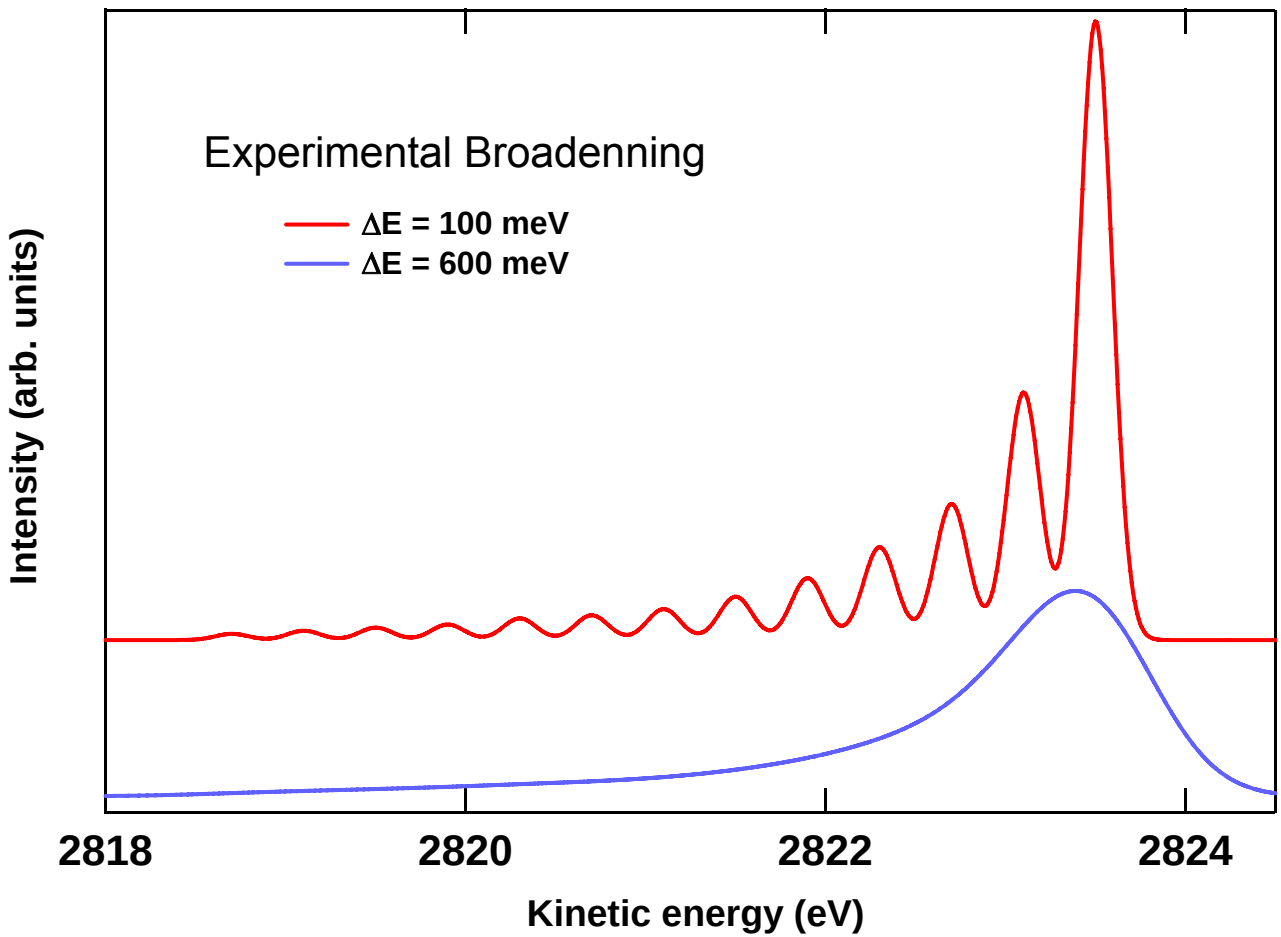
A common UHV chamber and analyser equipped with a removable gas cell and a 5 axis manipulator.

Preparation chamber and sample transfert.

Unique HAXPES available for Gas Phase.

RIXS diffractometer will be used by Gas phase and Solid state on the GALAXIES beamline

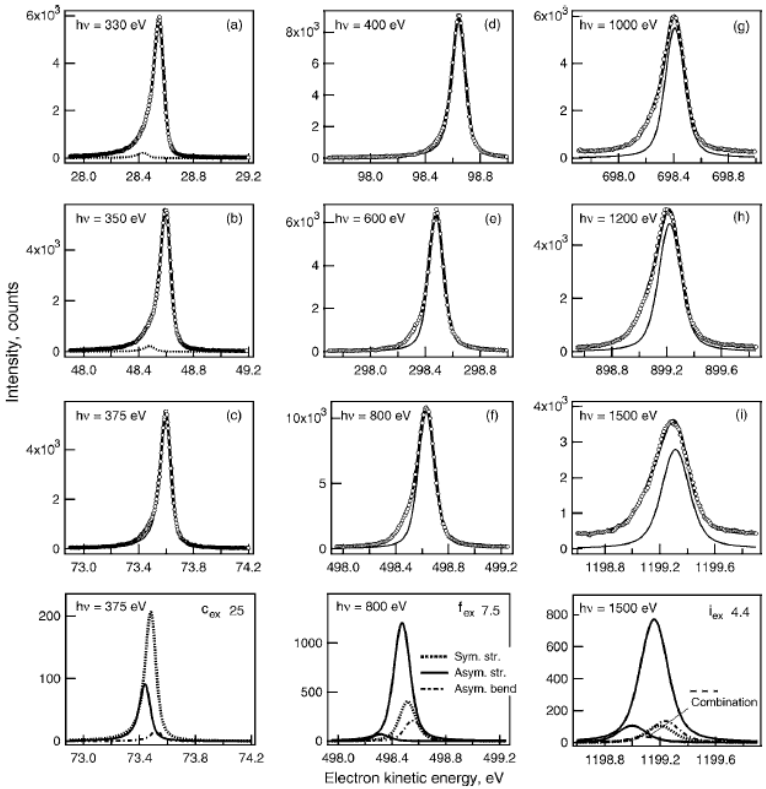
Vibrational progression allowing detailed nuclear motion



Recoil effect

Recoil excitation of vibrational structure in the carbon 1*s* photoelectron spectrum of CF_4

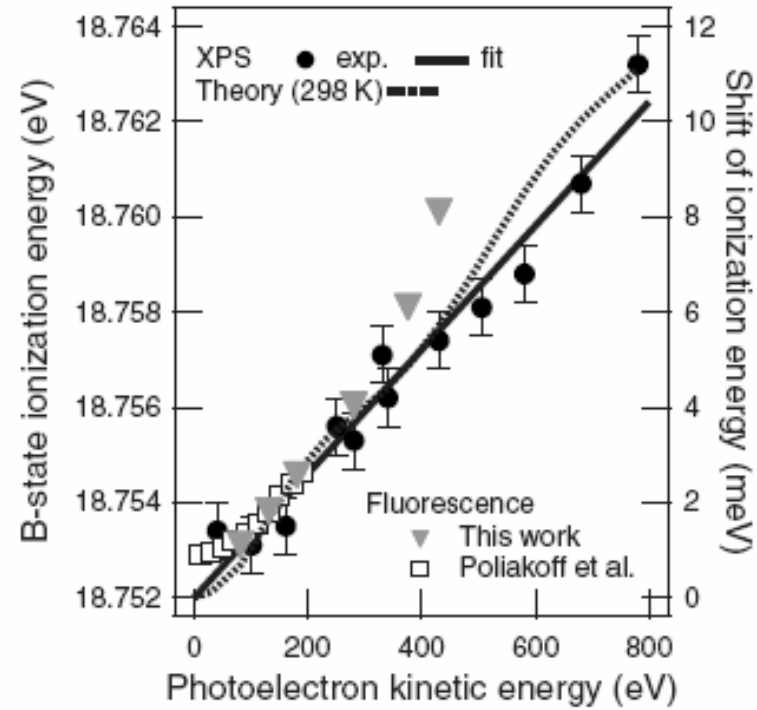
Localized character of core orbitals



Franck-Condon approximation not valid at high energy

T. D. Thomas et al., **J. Chem. Phys.** (2008)

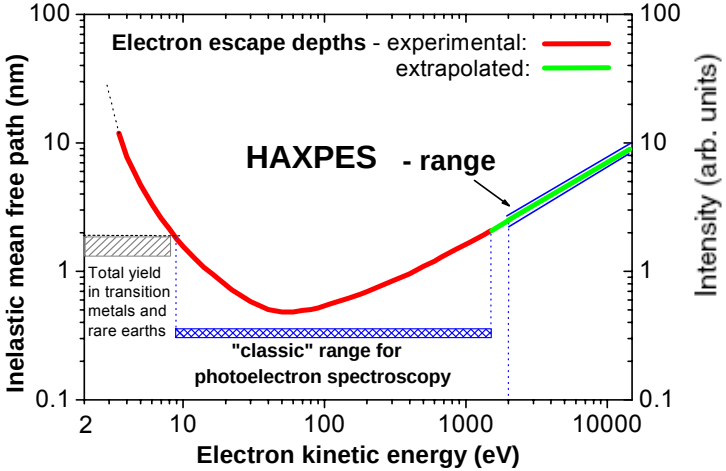
Recoil induced rotational excitation of the *B* state in N_2^+

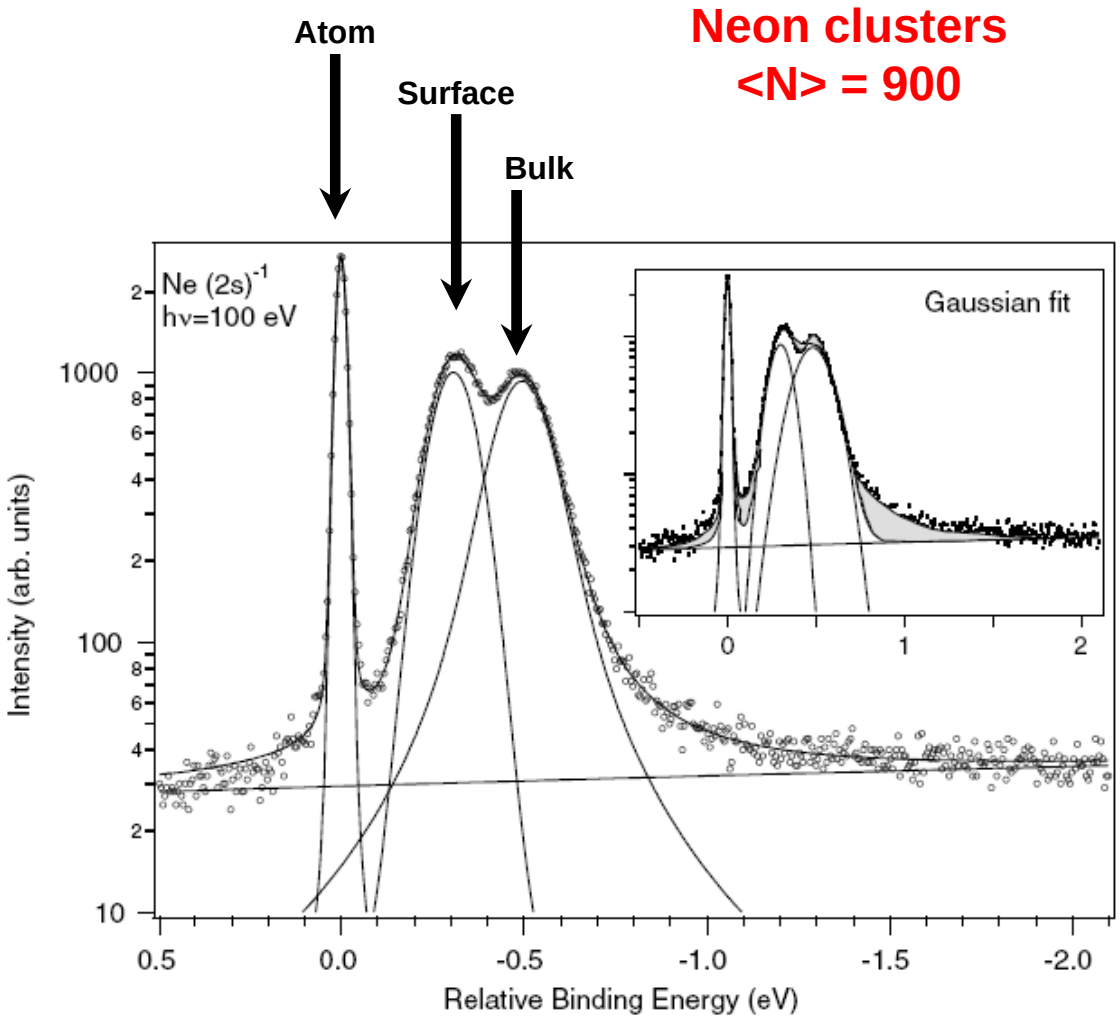


Mean apparent ionization energy to produce the *v*=0 *B* state of N_2^+ as a function of photoelectron kinetic energy. Solid circles, left-hand axis: From photoelectron spectroscopy.

T. D. Thomas et al., **Phys. Rev. A 79** (2009)

Structure determination of clusters





G. Ohrwall, M. Tchaplyguine, M. Lundwall, R. Feifel, H. Bergersen, T. Rander, A. Lindblad, J. Schulz, S. Peredkov, S. Barth, S. Marburger, U. Hergenhahn, S. Svensson, and O. Björneholm, Phys. Rev. Lett. (2004)

Galaxies beamline

- **Phase 2' beamline (mid 2010)**

- **U20 undulator, energy Range : 2.2-12 keV**

- **Two modes of Focalization**:
  > High-Flux: 80×35 µm² (H×V) FWHM
  > Micro-Focus: 5×5 µm² (H×V) FWHM

- **Scientific case: RIXS / HAXPES**
  ➢Strongly correlated materials (3d metal), heavy Fermions compounds (4f / 5f elements)
  > Local electronic / chemical properties: complex materials
  > In-situ study: high pressure, chemistry
  ➢Diluted phases

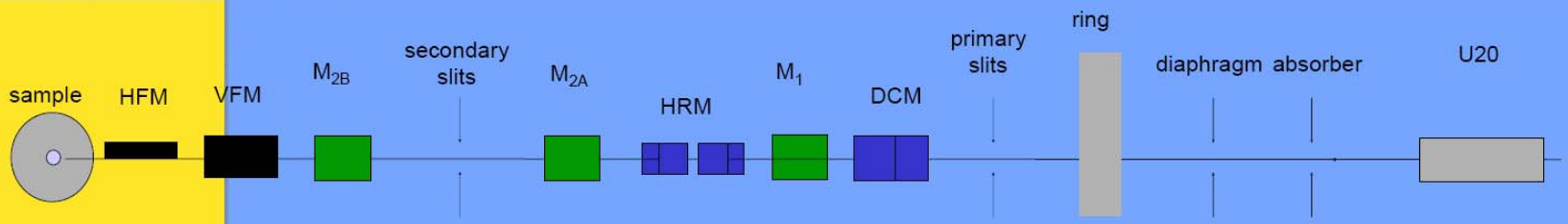
- **Ultimate resolution: Difractometer / Electron analyser**
  -200 meV at 8 keV of photon energy
  -35 meV at 12 keV of electron kinetic energy

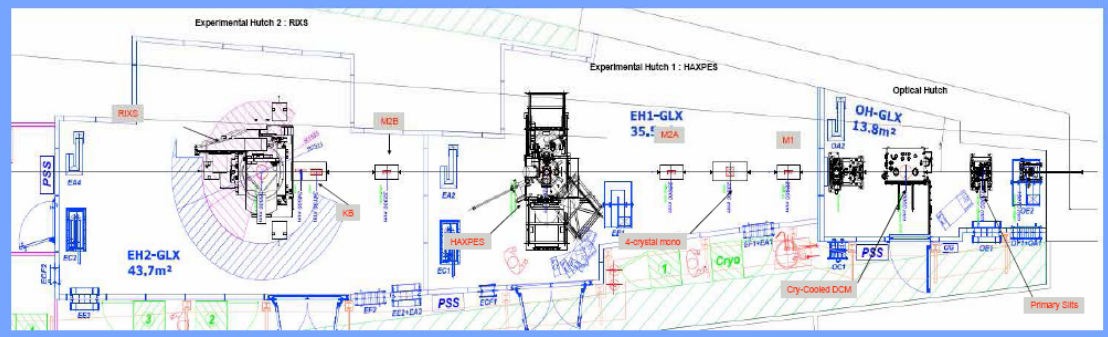
Characteristics

- U20, short section
- 2.3–12 keV, ΔE=50 meV – 1 eV
- Linear Polarisation
- Focalisation : 80 x 20 µm², 5 x 5 µm²
- Experimental end-stations:
  - **RIXS, HAXPES**

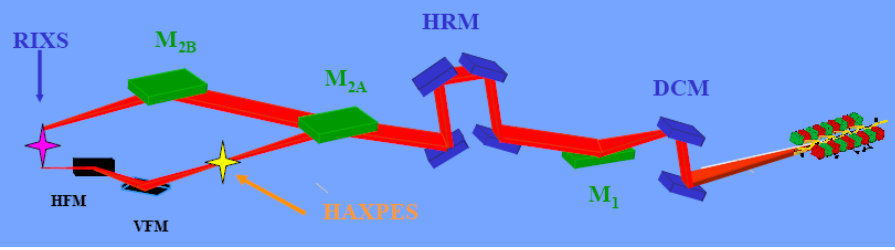
- Phase 2' beamline
- Operations in 2010

Top view



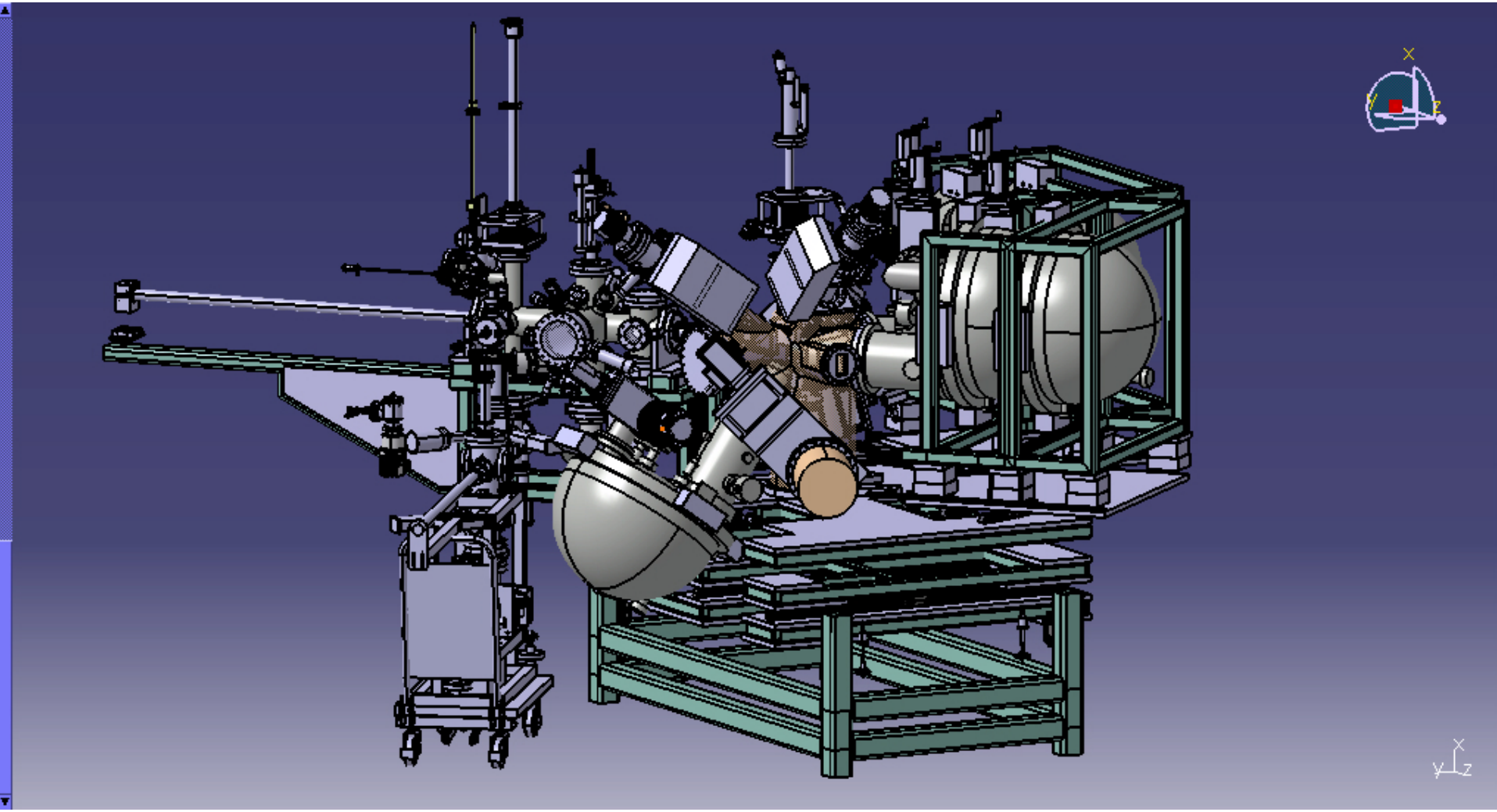


Beamline Layout



Resolution\focus	**Classical focus** 75×35 µm² (H×V) FWHM	**Microfocus** 14×9 µm² FWHM
without channel-cuts E/ΔE = 12000 à 6000	6×10^{13} ph/s	2×10^{13} ph/s
Si311 (n = 1) E/ΔE = 55000	6×10^{12} ph/s	2×10^{12} ph/s
Si220 (n = 2) E/ΔE = 150000	2×10^{12} ph/s	5×10^{11} ph/s

Electron analyser



HAXPES Workshop

SOLEIL 18-19th of January 2010

Svante SVENSSON: Chairman
Jean-Pascal RUEFF and Marc SIMON: Co-chairs