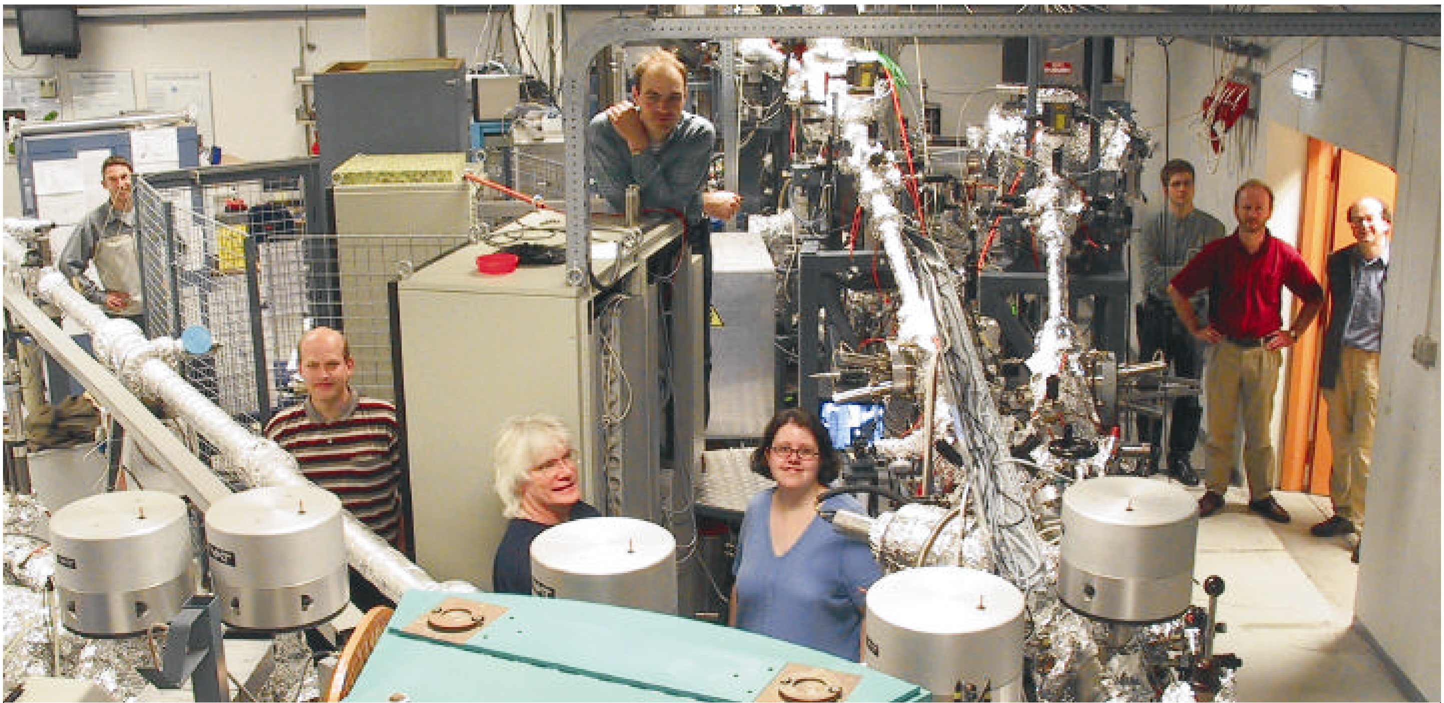
ISA

Institute for
Storage Ring Facilities
University of Aarhus

Newsletter No. 8 June 2001



The contributors to this newsletter standing in the undulator beamline area. From left to right they are: Peter A. Andersen, Søren Vrønning Hoffmann, John Kenney, Henrik Kjeldsen (on the platform), Nykola Jones, Philip Hofmann, Søren Pape Møller and David Field at the far right.

Present status of ISA *by Søren Pape Møller.*

Almost three years have passed since we last issued a newsletter. In this period, the research potential at our synchrotron-radiation facility has increased dramatically. Four world-class facilities within a broad research area, ranging from biology to astrophysics have been completed: an ultraviolet beamline for circular dichroism (CD) spectroscopy, and three undulator beamlines. These latter beamlines include experimental stations for 1) low-energy (meV) electron scattering on molecules, 2) photoionisation of ions in the 15-180 eV region, and 3) angular-resolved photo-electron spectroscopy on surfaces. Spectacular results have already been obtained, and in the present newsletter we will concentrate on these beamlines and some of the results.

Also the ion programme is very active, both at ASTRID and ELISA. One technical achievement at ASTRID has been the final commissioning of the Electron Beam Ion Source, which is now capable of delivering intense beams of highly charged ions; for example, currents in excess of 100 nA can be produced for Xenon for charge states up to 23. At ELISA, research with very heavy molecules of biological interest has been initiated. One example is lysozyme ions with a mass of approximately 15000 amu, which have been stored in ELISA.

During the period 1996-1999, ISA was funded from the Danish Research Ministry as a national laboratory. In this period the facilities at ISA expanded tremendously, for example with the introduction of the four beamlines mentioned above. In addition, new staff were hired. Since then, the funding for ISA has been reduced, partly because of the termination of the contract with the Research Ministry, partly because of a tight financial situation at the Faculty of Science. This has also resulted in a reduction of staff, and employees with high qualifications had to leave ISA. Their efforts are, however, highly appreciated.

The founder and previous director of ISA, Erik Uggerhøj has retired. Without Erik Uggerhøj's energy and engagement ISA would probably not have existed; at least not at the present level. He deserves great respect for all his accomplishments, and we wish him all the best in the future.

Finally, I am pleased to inform you that the proposal entitled *Access to the synchrotron radiation and ion storage facilities at the ASTRID accelerator complex* has been favourably evaluated by the European Commission under the programme *Improving Human Potential - Access to Research Infrastructures*. We are now in the process of contract negotiations.

Søren Pape Møller *fyssp@ifa.au.dk*

Low energy electron-molecule scattering experiments

by David Field and Nykola Jones

Laboratory astrophysics at ASTRID.

When sunlight falls upon the atmosphere of the earth, when starlight falls upon the interstellar medium, or when you turn on a light switch, a gas plasma forms containing electrons, molecules and positive ions. Electron-molecule collisions are fundamental to an understanding of the chemical and physical nature of gas plasmas, both natural and man-made. Plasmas range from those in space, for example around hot stars in our own or other galaxies or in the early Universe, to those in planetary atmospheres, especially that of the Earth, and to the chemically rich discharges used in industrial plasma processing.

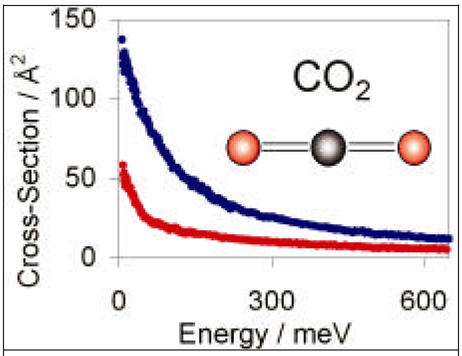
The CFH Telescope at the summit of Mauna Kea, Hawaii

Electrons turn out to be very effective in causing molecules to become excited and may also cause them to dissociate into neutral and negative ion products. To give some examples, ozone or chlorine dioxide may dissociate at specific electron impact energies to give negative ions. Molecules such as CCl_4 or SF_6 can capture electrons very efficiently and extinguish flames. The scattering properties of chlorine are important in determining the characteristics of chlorine-containing discharges, used in plasma and reactive ion etching in the fabrication of microchips.

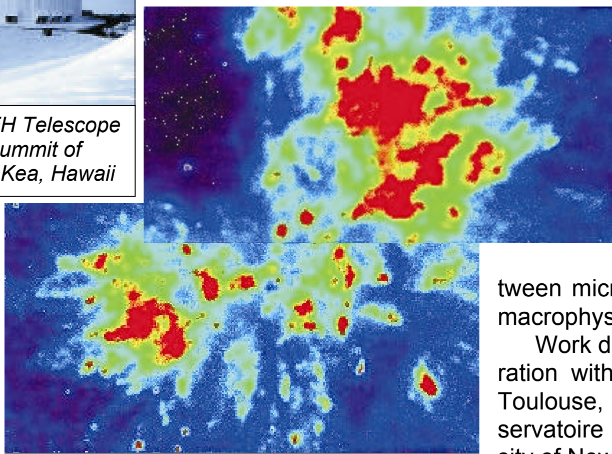
The motivation for our work is to gain physical insight into the nature of the strongly quantum-dominated collisions of electrons with molecules in the thermal energy range between a few tens to a few thousand degrees Kelvin.

In our experiments we make electron beams at low and well-defined energies with the ASTRID storage ring, using a high resolution monochromator on the ASTRID undulator beamline (SGM2). The principle is straightforward: synchrotron light interacts with argon gas at an energy of 15.75 eV (78.65nm) just above the photoionisation threshold. Photoelectrons are emitted with an energy of a few milli-electronvolts, that is, a few tens of Kelvin. The energy resolution of the electrons is given by the energy resolution of the photon beam and can be as good as 0.75 meV. A beam of electrons passes through a chosen target gas, and the attenuation of the beam as a function of electron kinetic energy is measured by continuously recording the electron current. These data allow us to derive the variation of scattering cross-sections with electron energy. An example of recent data is shown in the figure for carbon dioxide. These data allow us to identify experimentally for the first time a new and fundamental class of phenomena in which molecules interact strongly with electrons at very low energy through "virtual state scattering".

An area in which we can use our electron-molecule scattering data is in the study of star formation. Observations of the infrared emission of H_2 in Orion, using the Canada-France-Hawaii Telescope (see illustration), the European Southern Observatory 3.6m and the Very Large Telescope (Chile) show emission of vibrationally hot H_2 from dense self-gravitating clumps (see illustration). These clumps are candidate precursors to stars and are formed by plasma compression from a 200 km/s outflow from a nearby massive star in the Orion molecular cloud.



The variation of the integral (·) and backward (·) scattering cross-section of CO_2 by electrons.



Emission of vibrationally excited hydrogen at a wavelength of 2.121 mm in the Orion Molecular Cloud, 1500 light years away. Data obtained using the CFH Telescope.

Our experimental data for virtual state scattering are important in analyzing the density of gas in the clumps of H_2 seen in Orion and are part of the key to interpreting the brightness of the H_2 emission in terms of the pressure in the gas clumps. This example nicely illustrates the relationship between microphysics in the laboratory and macrophysics in the natural Universe.

Work decribed is conducted in collaboration with the University Paul Sabatier, Toulouse, University College London, Observatoire Paris-Meudon and the University of Newcastle-on-Tyne.

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Circular Dichroism Spectroscopy

by John Kenney and Søren Vrønning Hoffmann

From Parkinson's disease to spider silk: A wide range of biomolecules are studied on ISA's new UV beamline.

ISA's newest beamline, UV 1, has been designed to cover the ultraviolet and visible region from 700 nm to 100 nm, a biologically important wavelength region. UV 1 fills a gap in the range of wavelengths available at ISA.

The monochromator accepts radiation from a bending magnet, and provides a high flux (up to 10^{12} photons/sec.) with a moderate resolving power (>1000). The beamline consists a toroidal premirror, an entrance slit, a toroidal grating, and an exit slit. The choice of toroidal optics permits both horizontal and vertical focussing, while only reflecting the beam in the vertical direction. The latter is important, since this optical setup preserves the high degree of linear polarisation of the synchrotron radiation.

The high degree of linear polarisation, and the high flux makes this beamline particularly well suited for circular dichroism (CD) spectroscopy of optically active macromolecules. The ultraviolet region below 200 nm is very important for CD. At these short wavelengths commercial CD spectrometers suffer from a lack of flux.

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Spider silk is the world's toughest fibre. With obvious commercial importance, research at ISA is focused on understanding the molecular mechanism for its production. Already novel information has been revealed that is relevant to the material and to the medical sciences.

Angle-resolved photoemission spectroscopy *by Philip Hofmann*

Bulk bismuth is a poor metal, but the (110) surface of Bi is a good one.

One of the most fascinating aspects in the study of surfaces is the effect of reduced dimensionality on the electronic structure. It can lead to a situation where the surface has electronic properties, which are very different from those of the bulk material. In the bulk electronic structure of bismuth, for instance, there is only a very small overlap between the valence band and the conduction band. This causes Bi to be a poor metal, on the verge of being a semiconductor with an indirect band gap. Only a small change in the co-ordination of the Bi atoms can be expected to disturb this delicate balance such that a Bi surface could either turn into a better metal or into a semiconductor with a small, indirect gap.

Recently, the possibility of finding a metallic surface on rhombohedral Bi clusters has attracted some attention. It has been shown that granular systems built from small Bi clusters show superconductivity at rather high temperatures (up to several K) while pure bulk Bi is not a superconductor down to very low temperatures. A possible explanation of these findings is that localised electronic surface states could make the cluster surface more metallic than the bulk, a scenario that would favour the superconducting state.

In order to verify this, we have studied the surface electronic structure of the Bi(110) single-crystal surface, a surface which is also found on the clusters. In this experiment, the previously cleaned surface is cooled down to about 30 K and exposed to monochromatised light from ASTRID's SGM-3 undulator beamline. This leads to the photoemission of electrons from the occupied states in the sample. The experimental chamber contains an angle-resolved electron energy analyzer which can be moved in order to choose the emission direction and thereby the momentum of the detected electrons. The movement is achieved by two stepper motors outside the vacuum. It is controlled by a computer such that the analyzer can follow any desired path in momentum space.

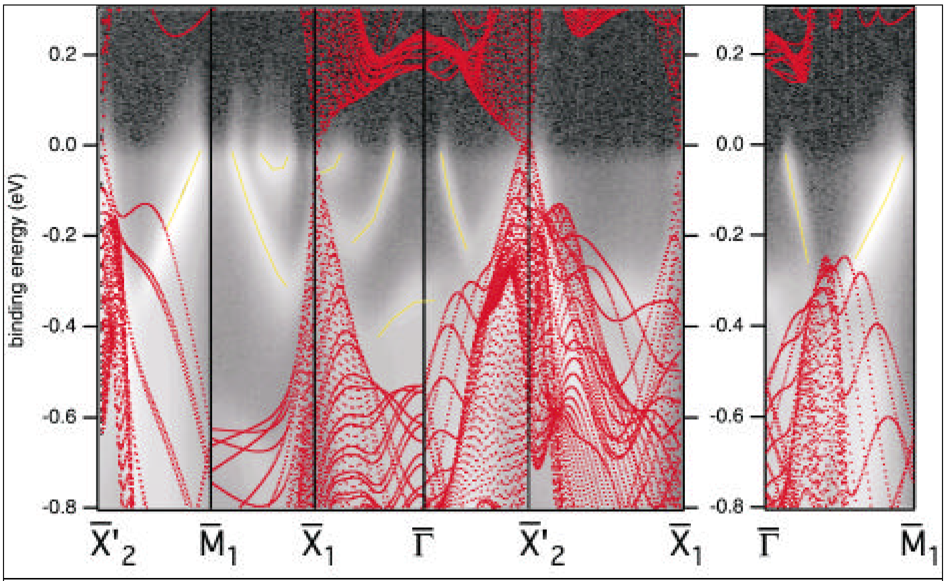

Figure 1: Photoemission intensity along some high symmetry lines of the Bi (110) surface together with a prediction for the electronic bulk states (red dots). The yellow lines emphasise the electronic surface states.

Figure 1 shows the photoemission intensity along several directions in reciprocal space (the greyscale image) together with a prediction for the bulk electronic structure (the red dots). One criterion for identifying a genuine surface state is that it does not fall into the area of the bulk

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CD-spectroscopy *continued from page 2*

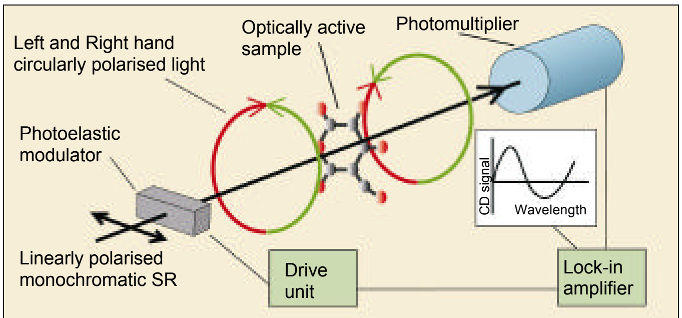
Synchrotron radiation sources on the other hand maintain their high flux levels throughout the UV and visible making them ideal for such studies.

The beamline, including the CD setup, was commissioned in October 2000, and upgraded in February 2001. Since then it has been used intensively, especially for CD, attracting users from many different institutions.

CD takes advantage of the intrinsic chiral nature of biomolecules using the differential absorption of left- and right-circularly polarised light to detemine the secondary structure content of proteins and nucleic acids. Using CD spectroscopy, molecular stability and conformational changes can be studied as a function of environment as well as folding and unfolding processes under normal and abnormal physiological conditions.

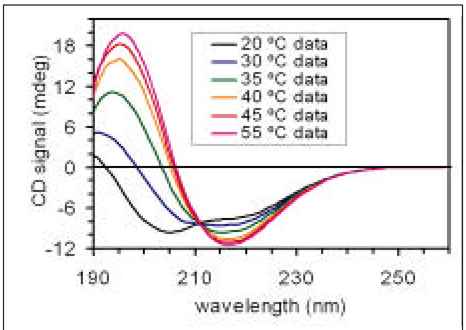
A significant role for CD follows on from the human genome project, especially in the field of functional genomics. CD can be used to rapidly characterise the gene products (i.e. proteins) over a wide range of conditions, and is particularly important in studying the relationship between the protein's structure and function.

Future developments and projects could include: CD microscopy, fluorescence CD, stop-flow/continuous flow CD, building a CD data base. Specific research areas cover a wide range of topics, from short peptides (too small to be properly considered proteins) to huge (700 kDa) proteins and DNA.



The principle of CD : By means of a polarisation modulator locked to the photomultiplier signal, the difference in right and left handed absorption can be measured.

A particularly interesting field of study involves the medically important amyloids of nervous disorders such as Parkinson's disease. Several projects have already been initiated to study these and related fibrilogenic protein systems, such as spider silk. As the world's toughest fibre (stronger than steel) it is of obvious commercial importance. Furthermore, research at ISA has already helped to shed light on the molecular mechanism underlying the formation of silk in the spider, indicating an unpredicted relatedness to disease amyloid formation.



Spectrum of silk temperature induced transition.

To learn more about CD at ISA, visit *www.isa.au.dk/SR/UV1/cd-spectroscopy.html* or contact John Kenney *kenney@ifa.au.dk*

Inner-shell photodetachment of Li^-

by Henrik Kjeldsen

First inner-shell photodetachment spectrum of a negative ion.

The negative ions form a special class of atomic systems with properties markedly different from those of neutral atoms and positive ions. They are characterised by an extremely strong correlation of the outer electrons, and therefore play an important role as fundamental test objects within atomic physics. As a consequence, they have been intensively studied in recent years. The use of lasers in photodetachment experiments has proved especially successful for mapping the properties of these exotic systems.

The photodetachment experiments, however, have been limited to the outer electrons, with no results reported for inner-shell photodetachment, simply due to the lack of an appropriate photon source. Lasers produce very intense beams, but only with photon energies that are low (typ. < 5 eV) compared to the binding energies of inner-shell electrons (typ. > 40 eV), and other photon sources cannot supply the required intensity.

Fortunately, the situation has recently changed. The undulator in the ASTRID storage ring delivers a very intense beam (more than 10^{13} photons pr. second) of photons with appropriate energies, 15 - 200 eV. By overlapping this beam with a beam of ions and detecting the resulting yield of photoionised ions it has become possible to measure absolute cross sections for photoionisation of ions. The set-up (figure 1) is quite complicated and consists of the ASTRID undulator, a Miyake monochromator, a small ion accelerator and equipment for analysis and detection. However, since all parameters are integrated into the ASTRID Control System the experiments can be controlled from a single PC. The set-up has already been used successfully to measure absolute photoionisation cross sections for positive ions (atomic and molecular) and recently also to record the first inner-shell photodetachment spectrum of a negative ion.

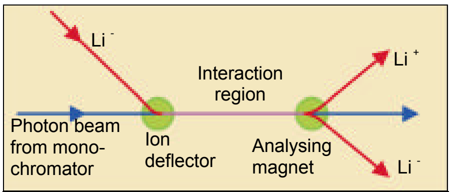


Figure 1: Setup (schematic).

Li^- was chosen as the target for the first experiment of this kind. The Li^- ion has the ground-state electron configuration $1s^22s^2$, and it is the lightest negative ion with a closed inner shell (the 1s shell). It is consequently an ideal candidate from a theoretical point of view and can be considered as a benchmark system for inner-shell photodetachment studies (in the same way as H^- is a benchmark system for outer-shell photodetachment studies).

The experiments on Li^- were rather difficult: It was only possible to obtain a density of Li^- ions in the target ion beam of about 1000/cm^3, and the only reason for success was the high photon flux available. Photodetachment of a 1s electron generally results in a core-excited Li state (plus a free electron), yet such a core-excited state will subsequently emit a so-called Auger electron and thereby decay to Li^+. The experiments were therefore performed by measuring the yield of Li^+ as a function of the photon energy.

The recorded spectrum (figure 2) is completely different from anything previously observed for any neutral atom or positive ion. The first thing that catches the eye is the intense peak around 60 eV. This peak is the result of $1s^22s^2 \rightarrow 1s2s2pns$ and $1s^22s^2 \rightarrow 1s2s2p + \varepsilon s$ transitions. The special thing is that these

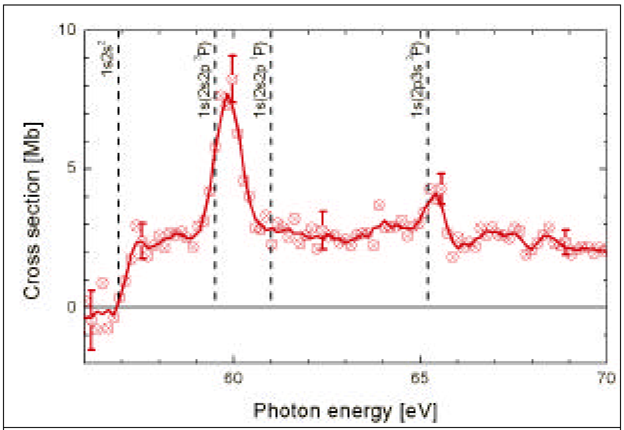


Figure 2: Photodetachment spectrum of Li^-.

are two-electron transitions: In neutral atoms or positive ions such features are usually much weaker than features due to one-electron transitions. But in the case of Li^- this is the dominating feature - a clear indication that the correlation of the electrons plays an extremely strong role. Note also that the peak is located above the corresponding limit $1s(2s2p\ ^3P)$ as indicated in the figure. This is another special feature for negative ions: The 1s2s2pns states are unbound (i.e. located above the corresponding limit) and therefore result in a so-called shape resonance instead of a Rydberg series of autoionising resonances converging to the limit as observed for atoms and positive ions.

In conclusion, the dominating feature is the peak at 60 eV, followed by the peak at 65 eV, whereas there is no peak above the first 1s limit ($1s2s^2$). This is somewhat surprising (and in strict contradiction with recent highly sophisticated calculations) since the first limit corresponds to a one-electron transition.

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Angle-resolved photoemission spectroscopy

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states, i.e. in the region of the red dots. In the figure, several such states can be identified (emphasised by the yellow lines). Some of them cross the Fermi level, i.e. the highest occupied level at 0 eV binding energy, and render the surface metallic.

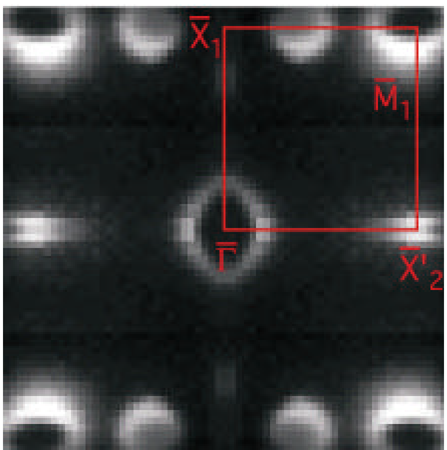

Figure 2: Photoemission intensity at the Fermi level in reciprocal space.

An even clearer impression of the surface metallicity is given in figure 2. It shows the photoemission intensity at the Fermi level in reciprocal space, i.e. it is a direct measure of the surface metallicity. All the features except the one close to the $\bar{X}'_2$ are surface related, and can be linked to the Fermi level crossings in figure 1.

This study shows that the (110) surface of Bi is a much better metal than the bulk, a fact which could explain the occurrence of superconductivity in granular systems built from small Bi clusters.

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