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ABSTRACT

We present a fully operational near-ambient pressure angle-resolved photoemission spectroscopy (NAP-ARPES) setup for operando studies of surface band structures under gas exposure at the TEMPO beamline of Synchrotron SOLEIL. The system integrates a SPECS PHOIBOS 150 NAP analyzer with multi-stage differential pumping and precise sample manipulation, enabling momentum-resolved electronic structure measurements under conditions approaching realistic environments. Commissioning experiments on graphite, ZnO(10-10), Cu(111), and Ru(0001) demonstrate operando capabilities, including reversible hydrogenation and adsorbate-induced modifications to the band structure. By bridging the gap between conventional UHV ARPES and operando surface science, this development provides a robust platform for investigating catalytic surfaces, energy conversion materials, and reactive interfaces under near-ambient conditions.

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I. INTRODUCTION

X-ray Photoelectron Spectroscopy (XPS) has long been a routine surface analysis technique providing elemental and chemical state information with high surface sensitivity. Over the past few decades, by bridging the pressure gap, Near Ambient Pressure XPS (NAP-XPS) has extended this ability to more realistic environments at pressures of a few millibars.^{1–7} Even pressures

beyond that have been realized using High-Energy X-ray Photoelectron Spectroscopy (HAXPES).⁸ The range of applications is broad, encompassing, among others, *in situ* studies of catalytic reactions,⁹ electrochemical interfaces,¹⁰ and gas-solid/liquid-solid/gas-liquid interactions.¹¹ This has made NAP-XPS a very valuable tool.

Nevertheless, NAP-XPS is limited to core-level spectroscopy and does not provide direct access to the electronic band structure, which is essential, i.e., for understanding charge transport,

surface states, and many-body interactions in functional materials. Angle-Resolved Photoemission Spectroscopy (ARPES) fills the gap by giving access to the momentum-resolved electronic structure. However, ARPES has traditionally been considered incompatible with near-ambient-pressure regimes (see, for example, Ref. 12) since the mean free path of photoelectrons in gas is extremely small, resulting in extensive scattering and loss of spectral resolution.

However, ARPES has long demonstrated its capability for probing adsorbate-surface interactions under high-vacuum to ultra-high-vacuum (UHV) conditions (see, for example, Refs. 13–17). For systems under atmosphere, a notable contribution came from the study of Ag–O₂ interactions using NAP-UPS, which highlighted the sensitivity of NAP-PES to subtle surface chemistry.¹⁸ Therefore, the next consequent step is operando near-ambient pressure ARPES—observation of electronic structure during surface reactions in a gas atmosphere. This is particularly valuable when handling catalytic surfaces, energy-conversion materials, and low-dimensional systems in which surface interactions are a key factor. NAP-ARPES naturally complements NAP-XPS by incorporating the momentum-resolved information and delivering a more complete picture of surface processes under more realistic conditions. Early demonstrations of this approach were presented at the NAP-XPS endstation of beamline 9.3.2 at the Advanced Light Source,⁵ showcasing NAP-ARPES capabilities with graphene under 0.25 mbar CO-gas. However, the system lacked a full-featured sample manipulator for precise angular alignment, making it more of a proof-of-concept than a fully operational NAP-ARPES setup.

This paper presents a *fully operational* Near Ambient Pressure ARPES (NAP-ARPES) system established for user operation at the TEMPO beamline at Synchrotron SOLEIL, where a commercial SPECS NAP-XPS system is supplied by photons in the XUV and soft x-ray regime (50–1500 eV). The commercial electron analyzer was equipped with differential pumping, and a gas-handling system was upgraded with a custom-designed electron lens, enabling ARPES measurements at relatively high pressures, meaning up to a few mbar at the sample. The systems' functionality is demonstrated by NAP-ARPES on graphite (HOPG), ZnO(10-10), Cu(111), and Ru(0001) exposed to mbar pressures of representative gases, in some

cases leading to pronounced but selective changes in the band structure. This development is thus a further step in the quest to close the long-standing pressure gap between idealized UHV-based and real-world surface science and provides avenues for future research in catalysis, energy materials science, and reactive interfaces under more realistic conditions.

II. TEMPO BEAMLINE BRANCH B

The basic optical setup of the TEMPO beamline at SOLEIL is described in Ref. 19 and is displayed in Fig. 1. It employs two APPLE II undulators with magnetic periods of 80 and 44 mm, enabling a wide energy range from 50 to 1500 eV. This configuration provides full polarization control (linear and circular) over the full energy range, which is essential for magnetic and orientation-sensitive experiments. The monochromator uses plane gratings with Variable Line Spacing (VLS) and Variable Groove Depth (VGD) for vertical focusing. Depending on photon energy, grating selection, and slit settings, the beamline provides a resolving power exceeding 10 000 and a photon flux at the sample of up to 10^{15} photons/s/0.1% bandwidth under optimized conditions. In practice, however, photon flux and energy resolution cannot be maximized simultaneously. For the NAP-ARPES measurements presented here, the beamline was intentionally operated using a compromise between count rate and spectral resolution suitable for near-ambient-pressure experiments. As a reference, energy resolutions of ~ 15 meV at 100 eV photon energy with flux suitable for ARPES measurements and about 80 meV at 700 eV under typical XPS operating conditions can be achieved. The performance values reported in this work, therefore, reflect the actual experimental settings rather than the maximum beamline specifications.

Branch B incorporates a switching mirror after the exit slits to redirect the beam toward the secondary experimental station. This branch is dedicated to NAP-XPS and NAP-ARPES experiments. A fast valve between the switching mirror and the NAP-entrance ensures vacuum safety during near-ambient pressure experiments.

The soft x-ray beam enters the analysis chamber through a windowless beamline entrance equipped with a three-stage differential-

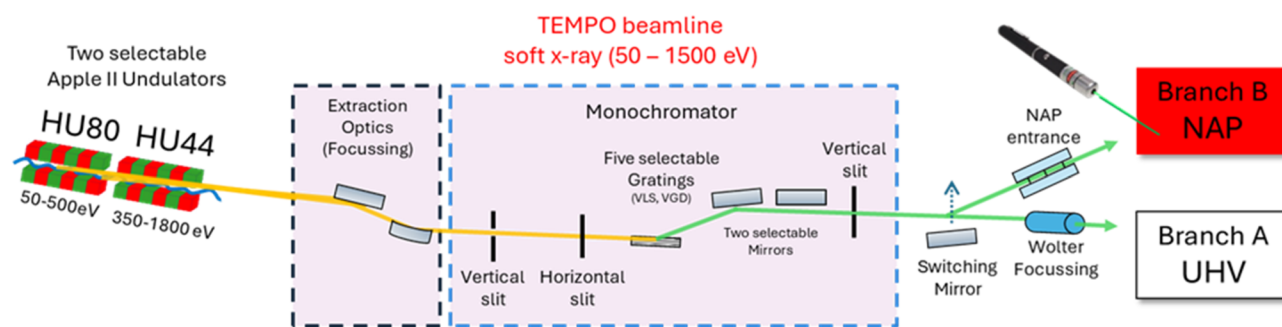


FIG. 1. Schematic optical layout of the TEMPO beamline. Starting from the left, two APPLE II undulators with magnetic periods of 80 mm (HU80) and 44 mm (HU44) generate the incoming radiation. The light is first collected by the initial pair of extraction optics and then passes through a vertical slit (closing in the vertical direction) followed by a horizontal slit. The monochromator stage consists of four selectable gratings (VLS/VGD). To satisfy the Rowland mounting conditions over the full energy range, two interchangeable mirrors are positioned downstream of the gratings and upstream of the exit slit. Finally, a switching mirror directs the monochromatized beam toward one of the two endstations. The endstation described in this work corresponds to Branch B, equipped with the near-ambient-pressure (NAP) setup.

pumping system. This differential pumping system uses a sequence of progressively smaller pinholes, ending with a 300- μm -diameter capillary on the chamber side. Each stage is pumped independently, allowing the ultra-high-vacuum conditions required by the beamline optics to be maintained while the analysis chamber is operated at pressures of up to several millibars. In addition, a fast-closing valve is installed between the beamline and the endstation. In the event of a failure of the differential pumping system or an unexpected pressure excursion, this valve automatically isolates the beamline within a few milliseconds, thereby protecting the upstream optics and storage-ring vacuum. Such a design avoids any window-related absorption losses, which would otherwise be significant at low photon energies (<100 eV), and is, therefore, essential for NAP-ARPES.

After the beamline entrance follows the NAP-PES endstation at Sorbonne Université, which is described below. The beam impinges at an angle of 54° relative to the analyzer axis.

III. NAP-PES ENDSTATION

The overall layout of the NAP-PES endstation is summarized schematically in Fig. 2. As illustrated in Fig. 2, the endstation comprises three UHV-compatible chambers with a base pressure in the 10^{-9} – 10^{-10} mbar range: (i) a μ -metal analysis chamber hosting the SPECS PHOIBOS 150 NAP analyzer, (ii) a preparation chamber equipped with an ion gun, LEED, and multiple auxiliary ports for devices such as a quartz microbalance and evaporators, and (iii) a high-pressure treatment chamber capable of pre-treatments up to 1 bar. Consistent with the differential pumping scheme highlighted in Fig. 3, the pressure in the analysis chamber can be tuned continuously between 10^{-9} mbar and 20 mbar. Pressure regulation is ensured through leak valves and monitored using a capacitance

manometer, while a fully automated gas-handling system provides precise control over gas-mixture compositions.

Two sample environments are available. In the first configuration, an AIN button heater allows temperature variation from ambient conditions to 600 K under measurement conditions. In the second configuration, a Peltier module enables temperature control from ambient conditions down to -10°C .

IV. SPECS PHOIBOS 150 NAP ANALYZER OPTIMIZED FOR ARPES

A. Spectrometer overview

The use of electrostatic focusing combined with differential pumping to enable photoelectron spectroscopy in the millibar pressure range was pioneered by Ogletree *et al.* through the development of a differentially pumped electrostatic lens system for ambient-pressure photoemission.⁷ Subsequent implementation in a dedicated ambient-pressure photoemission endstation further established this concept as the foundation of modern NAP-XPS instrumentation.²⁰

The SPECS PHOIBOS NAP analyzer at TEMPO, depicted at the core of the analysis chamber in Fig. 2, features four differentially pumped stages. Its wide-angle acceptance pre-lens is separated from the main chamber by a 0.3 mm conical nozzle; see also Fig. 5(a). A quadrupole mass spectrometer (QMS) in the second pumping stage (see also Fig. 3) allows continuous monitoring of the gas-phase composition; here, the pressure is reduced by a factor of 10^4 compared to the analysis chamber. The working distance between the nozzle entrance and the sample surface is 300 μm . Thanks to the multi-stage differential pumping system (also schematically represented in Fig. 2 and labeled as beamline entrance), pressures as low as 10^{-8} mbar are

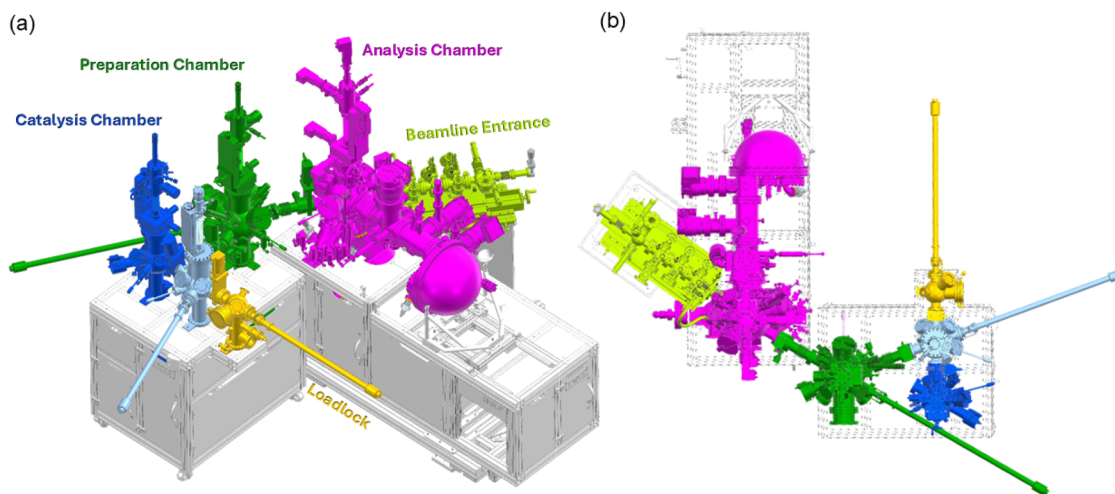


FIG. 2. Schematic overview of the Sorbonne Université NAP-PES endstation at TEMPO in (a) side perspective view and (b) top view. The system was designed by SPECS and comprises a load-lock and a transfer/storage chamber, followed by two dedicated preparation environments—a catalysis chamber and a preparation chamber, positioned upstream of the analysis chamber. At the core of the analysis chamber is the SPECS PHOIBOS 150 NAP analyzer. The beamline entrance remains open thanks to a three-stage differential pumping scheme, which preserves the soft x-ray beamline vacuum while allowing the analysis chamber to operate at pressures up to several millibars.

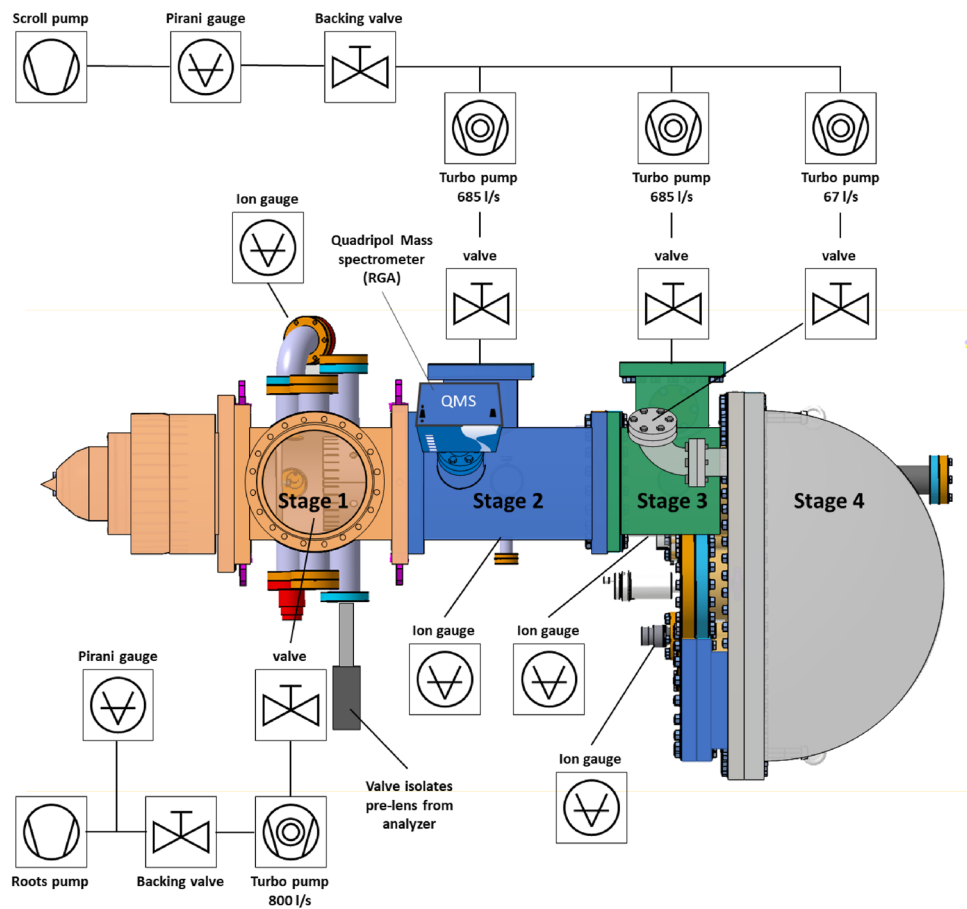


FIG. 3. Pumping scheme of the SPECS PHOIBOS 150 NAP showing the four stages. For details, see the text.

maintained in the detector section and at the beamline’s first mirror, even when the analysis chamber is operated at 20 mbar.

The central component of the NAP-XPS endstation is an upgraded SPECS PHOIBOS 150 NAP analyzer, a near-ambient pressure spectrometer equipped with a two-dimensional delay-line detector developed by Surface Concept, allowing simultaneous measurement of time, position/angle, and energy. The system features a true 180° hemispherical energy analyzer with a mean radius of 150 mm, coupled to a three-stage lens assembly. The pre-lens section incorporates an ellipsoidal mesh lens designed for a high acceptance angle. To ensure optimal performance, the analyzer and lens system are constructed entirely from non-magnetic materials and are enclosed within two layers of 2 mm-thick μ -metal shielding. This configuration effectively suppresses external magnetic fields to negligible levels.

The analyzer has eight selectable entrance slits at the entrance plane that are available in different shapes and sizes (straight, round, and curved). The available entrance slits are listed in Table I. On the detector side of the hemisphere are three exit slits. One exit slit contains an array of parallel slits used to verify the detector’s rotation. Another incorporates a mesh that shields the interior of the hemisphere from the detector’s bias voltage, which improves detection efficiency. The third slit is open and serves as the standard exit

TABLE I. Available analyzer entrance slits for the upgraded SPECS PHOIBOS 150 NAP spectrometer. Rectangular slits are specified by their width (w) and length (L), whereas circular apertures are specified by their diameter.

Slit No.	Analyzer entrance slits	
	Shape	Slit size
1	Rect. (w $\times$ L)	0.2 $\times$ 20 mm ²
2	Rect. (w $\times$ L)	0.5 $\times$ 20 mm ²
3	Rect. (w $\times$ L)	1.0 $\times$ 20 mm ²
4	Rect. (w $\times$ L)	3.0 $\times$ 20 mm ²
5	Rect. (w $\times$ L)	7.0 $\times$ 20 mm ²
6	Circ. (dia)	1.0 mm
7	Circ. (dia)	3.0 mm
8	Circ. (dia)	7.0 mm

for normal ARPES imaging operation to prevent the mesh structure from being visible in the images.

B. Differential pumping system

The spectrometer consists of a differentially pumped electrostatic pre-lens combined with a three-stage differentially pumped

PHOIBOS 150 EP analyzer. Together, they provide four distinct pressure stages separated by apertures. The pumping scheme is depicted in Fig. 3.

For efficient and targeted pumping, the electron optics is equipped with openings and sealed at appropriate positions using Viton O-rings.

The first stage (pre-lens) is separated from the analysis chamber by a conical entrance nozzle (aperture tip diameter between 0.3 and 2 mm); see also Fig. 5. With turbo pumping (800 l/s), a pressure reduction of four orders of magnitude compared to the analysis chamber can be achieved. Measurements for this are displayed in Fig. 4.

The second stage is isolated from the first stage by a conical aperture, 24 mm in length, with an inlet diameter of 8 mm and an outlet diameter of 5 mm, equipped with an in-lens gate valve, enabling a high-vacuum seal between the analyzer and the pre-lens. This design allows venting of the analysis chamber and pre-lens without venting the energy analyzer.

The third stage is positioned behind two iris apertures separating the front and rear electrostatic lens sections. The fourth stage houses the hemisphere and detector.

A key challenge for near-ambient-pressure operation is achieving efficient differential pumping, which must gradually reduce the gas load along the electron path. While this can in principle be accomplished by using smaller apertures, such a solution introduces limitations: electrostatic lenses and apertures at very small dimensions can significantly reduce transmission and degrade imaging performance if not carefully designed. The region between the first and second pumping stages, the conical aperture, is particularly critical in this regard. To overcome these constraints, the pre-lens electron-optical system was redesigned and optimized to ensure reliable NAP-ARPES measurements.

C. Electron optical design

The electron-optics simulations were performed using the SIMION ray-tracing package, a well-established program for charged-particle trajectory calculations.²¹ In summary, the program represents the electrode assembly with its defined geometry and symmetry on a two-dimensional potential grid. Grid points

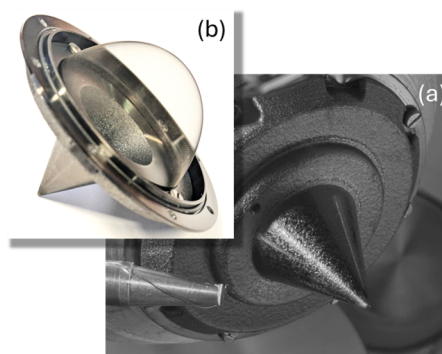


FIG. 5. Entrance nozzle with a 0.3-mm opening and a $\pm 22^\circ$ clearance angle, equipped with a high-transmission ellipsoidal mesh.

corresponding to electrode surfaces are fixed at their respective applied potentials. The electrostatic potential in the remaining (non-electrode) regions is then obtained through an iterative finite-difference relaxation procedure, in which each grid point is updated by averaging the potentials of its nearest neighbors. This process is repeated until self-consistency is reached and the desired numerical accuracy of the potential map is achieved.

The trajectory calculation algorithm then determines the motion of charged particles within the resulting electrostatic field by evaluating the electrostatic forces, numerically integrating the particle paths, and adjusting time steps as necessary. Consequently, the electron-optical characteristics of a system can be simulated for specified initial beam parameters, such as starting positions, launch angles, spatial distributions, and energy distributions.

The transfer optics are critical to the performance of the NAP electron spectrometer. The entrance nozzle, shown in Fig. 5, has a conical geometry with a 45° outer half-angle and a minimum orifice diameter of 0.3 mm. This configuration maximizes differential pumping efficiency, reducing pressure to the 10^{-3} mbar range within a few millimeters of the sample surface. The nozzle is modular and can be exchanged for variants with different aperture diameters to adapt to specific experimental requirements.

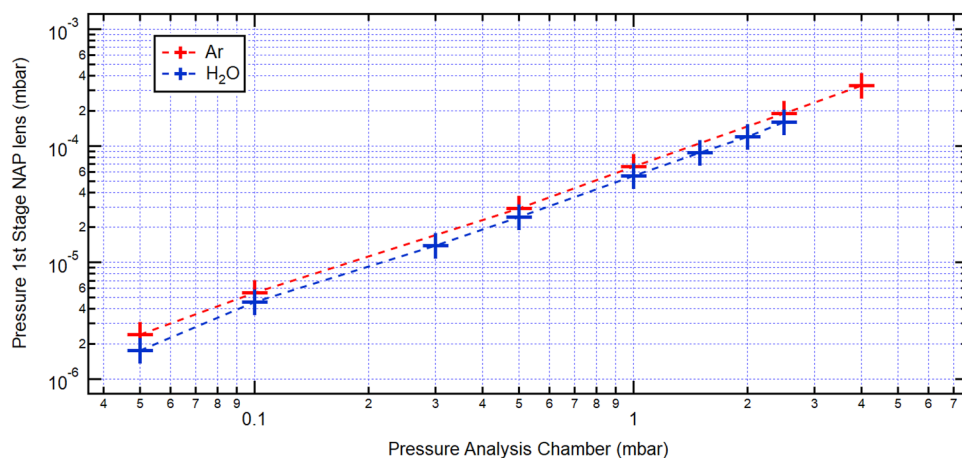


FIG. 4. Comparison of the pressures of the analysis chamber and first stage for Ar and H₂O showing almost a linear four orders of magnitude reduction in the relevant NAP pressure range.

The spectrometer supports multiple lens modes for both UPS and XPS applications. In this work, the ARM22 angular-dispersive mode is employed, in which the maximum acceptance angle of $\pm 22^\circ$ is spread along the 20 mm analyzer entrance slit.

In contrast to an angle-integrated lens mode, as employed in NAP-XPS, the primary objective of angular dispersive lens mode optimization for NAP-ARPES is to achieve linear angular dispersion and to prevent large-angle trajectories from being folded into the region of interest. In addition, the angular dispersion value must be adjusted so that the desired angular range is fully accommodated by the analyzer slit length. To minimize aberrations, the emittance angle at the lens exit plane, which coincides with the entrance plane

of the hemispherical analyzer, should remain below a critical threshold. The angular resolution can be calculated from the trajectory spread at the detection plane due to the finite spot size at the sample plane and the angular dispersion.

In electrostatic lens systems, trajectory shapes are governed by the ratios of the applied potentials rather than by their absolute values, reflecting the scaling invariance of the electrostatic equations of motion. In the present constant-pass-energy operation, the relevant scaling parameter is the retarding ratio, $RR = E_{\text{kin}}/E_p$. Accordingly, Fig. 6 illustrates the effect of changing lens conditions by comparing two representative operating points, $RR = 3.25$ and $RR = 5.0$, which cover the most relevant range used for the measurements discussed

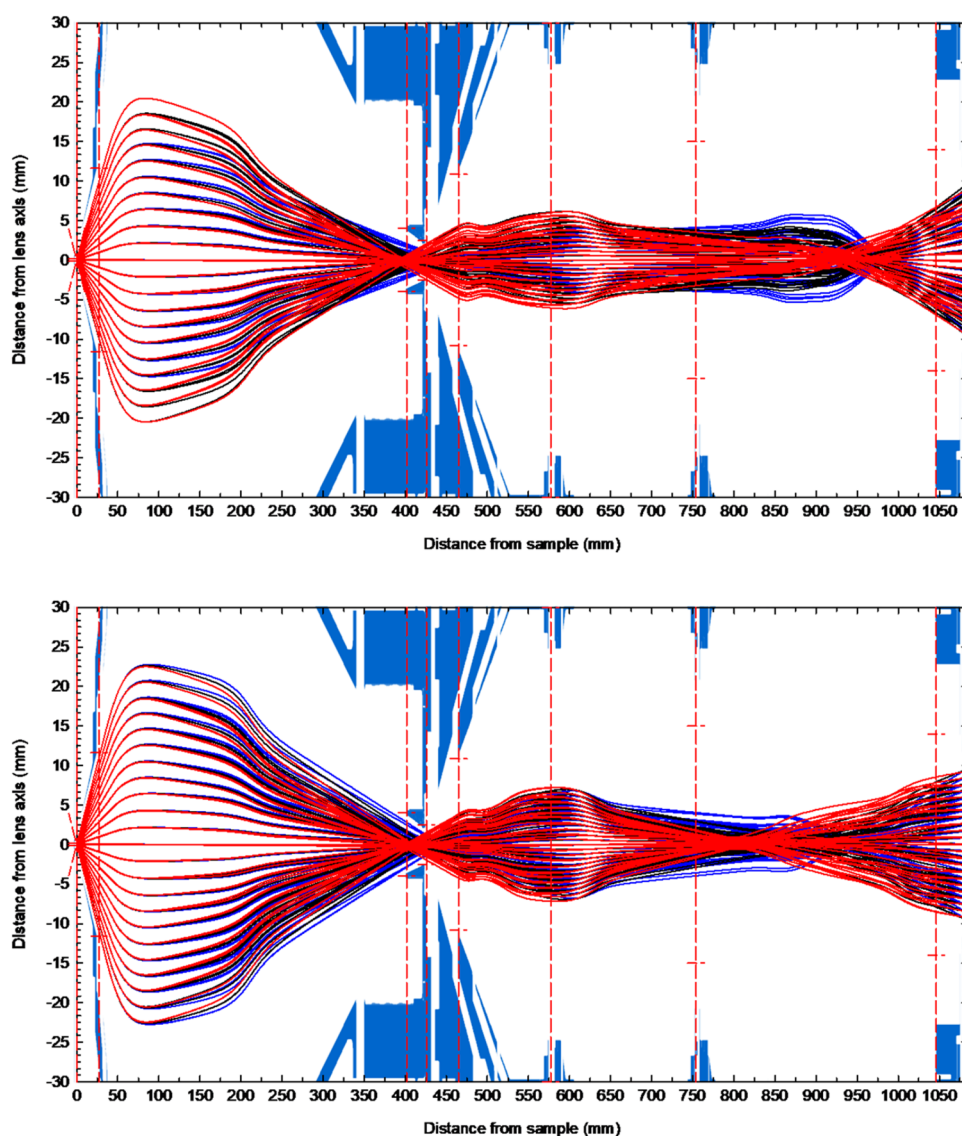


FIG. 6. Electron trajectories in the ARM22 mode at $E_{\text{kin}} = 65$ and 100 eV ($E_p = 20$ eV, $RR = 3.25$ and 5.0 , respectively). Trajectories span $\pm 0.03 E_p$, with red, black, and blue indicating $E_{\text{kin}} - 0.03 E_p$, E_{kin} , and $E_{\text{kin}} + 0.03 E_p$, respectively. The red dashed lines mark the positions and diameters of the lens apertures. The lens contour is illustrated by the blue shaded areas within the displayed region.

here. Figure 7 adds $E_{\text{kin}} = 430$ eV ($E_p = 100$ eV; $RR = 4.3$), covering the experimentally relevant operating range for the soft-x-ray ARPES of ZnO, also discussed in the following.

A comparison of the ray-tracing results at $E_{\text{kin}} = 65$ eV and $E_{\text{kin}} = 100$ eV, both at $E_p = 20$ eV, as shown in Fig. 6, reveals a characteristic performance limitation of mesh lenses at low retarding ratios, $RR = E_{\text{kin}}/E_p$. While at $RR = 5.0$, the angular resolution reaches 0.57° with 95.7% transmission, the angular resolution degrades noticeably at $RR = 3.25$. This degradation is not uniform: the central angular region remains well resolved, while aberrations increase toward the outermost acceptance angles. This behavior is inherent to mesh-type electrostatic lenses, which effectively suppress spherical aberrations, but exhibit pronounced chromatic aberrations at low retarding ratios.

This limitation can be mitigated by the SA2 lens mode, which applies an accelerating voltage to the conical transition electrode between the first and second lens stage, an element held at ground potential in the standard configuration.

Due to the lens's rotational symmetry, the entrance and exit segments of the trajectories correspond to the cross sections of cones defined by the electron angular distribution. When operating the spectrometer at constant pass energy, it is important to keep the lens mode properties constant over a large energy range. The trajectories shown here correspond to an energy range of $\pm 0.03 E_p$, with red, black, and blue representing the lower ($E_{\text{kin}} - 0.03 E_p$), central (E_{kin}), and upper ($E_{\text{kin}} + 0.03 E_p$) energy, respectively. Electrons with higher kinetic energy experience a weaker focusing action from the electrostatic lens field, resulting in focal points shifting further toward the

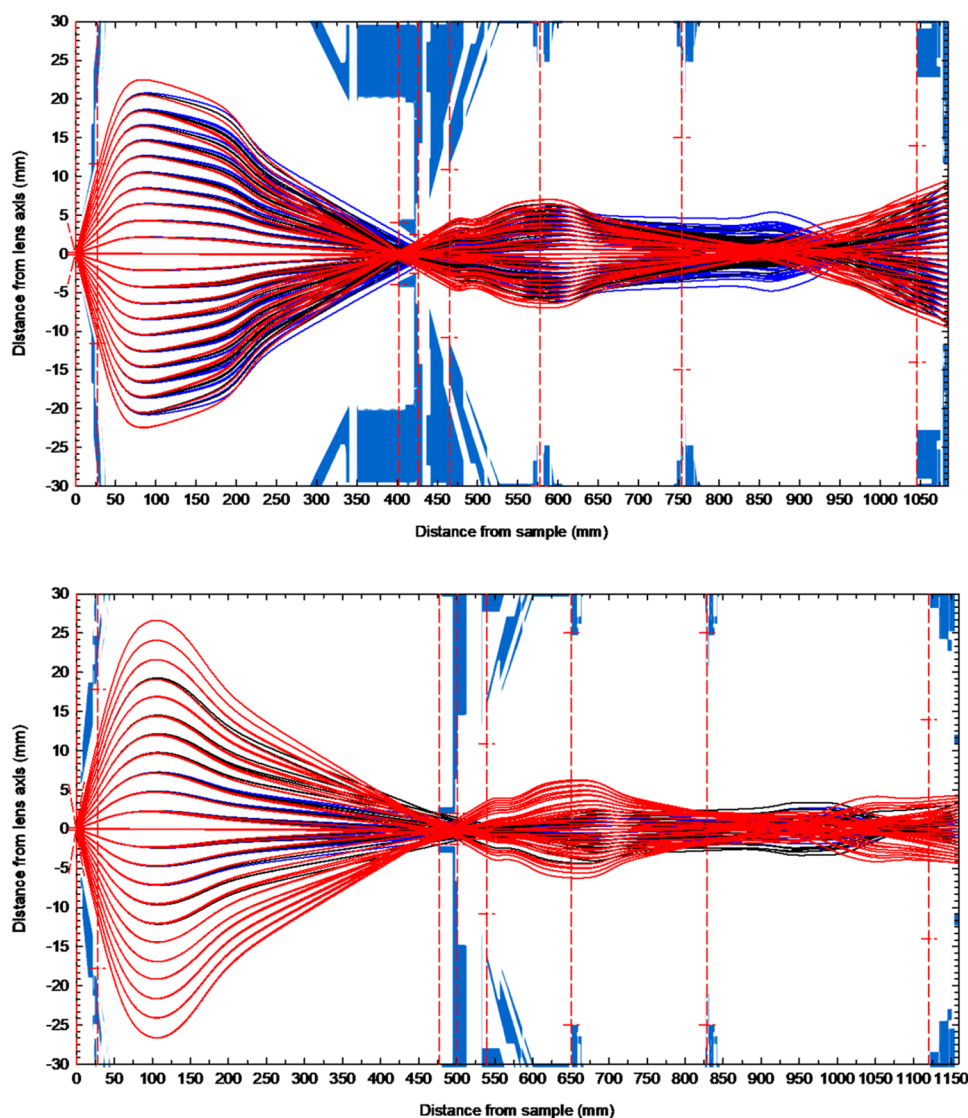


FIG. 7. Electron trajectories in the ARM22 mode for the upgraded (ellipsoidal mesh lens) and former (spherical mesh lens) lens system at $E_{\text{kin}} = 430$ eV ($E_p = 100$ eV, $RR = 4.3$). Trajectories span $\pm 0.03 E_p$, with red, black, and blue indicating $E_{\text{kin}} - 0.03 E_p$, E_{kin} , and $E_{\text{kin}} + 0.03 E_p$, respectively. The red dashed lines mark the positions and diameters of the lens apertures. The lens contour is illustrated by the blue shaded areas within the displayed region.

analyzer entrance compared to lower-energy electrons. The position and diameters of the lens apertures are indicated by the red dashed horizontal lines.

The redesign of the upgraded lens system comprises two key modifications affecting the first lens stage and the differential pumping transition. First, the electron-optical elements of the first lens stage were comprehensively redesigned: the mesh lens geometry was changed from spherical to ellipsoidal, and the subsequent focusing electrodes were re-optimized to match the modified beam envelope, improving collection efficiency and reducing aberrations across the relevant kinetic energy range. Second, the geometric transition between the first and second differential pumping stages was redesigned from a cylindrical to a conical geometry. This conical element reduces electron beam clipping at the stage boundary and improves the phase-space acceptance of the subsequent lens elements. It also serves as the accelerating electrode in the SA2 lens mode described above.

The upgraded lens demonstrates clear advantages over the former lens across all operating conditions relevant to NAP-ARPES. Transmission is consistently higher, directly translating into improved signal intensity at a given photon flux—a critical benefit under near-ambient pressure conditions where gas-phase scattering inherently reduces count rates. Linear dispersion increases by approximately a factor of two, providing better angular separation on the 2D detector and improving the effective band structure resolution. Most notably, at $E_{\text{kin}} = 100$ eV ($RR = 5.0$), the angular resolution improves significantly to 0.57° , indicating that the upgraded lens system performs reliably at lower retarding ratios than its predecessor.

The theoretically achievable energy resolution of the instrument, assuming zero angular spread ($\alpha = 0$) and a slit width w , is given by $w/(2R_0) \times E_p$.²² With $R_0 = 150$ mm and $w = 0.5$ mm (Slit No. 2 in Table I), this yields 33 meV for $E_p = 20$ eV and 167 meV for $E_p = 100$ eV. In practice, electrons enter the analyzer with a finite angular distribution α , which contributes an additional broadening

α -term and typically doubles the experimentally achievable energy width ΔE .

D. Determination of energy and angular resolution

The experimental energy and momentum resolution of the spectrometer was determined using the Shockley surface state of Cu(111). The clean surface was prepared by repeated cycles of Ar ion sputtering [$p(\text{Ar}) = 1 \times 10^{-5}$ mbar, $U = 1000$ V, $I_{\text{ion}} = 10$ mA, 10 min] and annealing (800 K, 10 min) and confirmed by LEED. All data shown in Fig. 6 were measured under UHV conditions at room temperature (300 K) using a photon energy of 70 eV.

Figure 8(a) shows the ARPES band map of Cu(111) acquired in the angular-dispersive ARM22 lens mode. To quantify the energy resolution, we display in Fig. 8(b) an energy distribution curve (EDC) extracted near the Fermi wave vector (at an emission angle of -2° , averaged over an angular window of $\pm 1^\circ$). The spectrum was fitted with a Fermi–Dirac function convoluted with a Gaussian broadening function. The resulting Gaussian full width at half maximum (FWHM) is 100 meV, which reflects the instrumental (beamline and analyzer) energy resolution.

The experimentally obtained value can be compared to the expected energy resolution of a hemispherical analyzer above. For $w = 0.5$ mm, $R_0 = 150$ mm, and $E_p = 20$ eV, we expect 67 meV. The experimentally observed energy resolution of 100 meV is, therefore, reasonably close to the analyzer-limited value, with the remaining broadening of around 70 meV attributed to the beamline optics at that setting. The latter value reflects the deliberately chosen high-flux operating mode used for the present NAP-ARPES measurements, rather than the maximum resolving power achievable at TEMPO. Note that the setting is optimized for realistic experimental conditions in terms of count rate vs resolution, following the principle that the resolution of the spectrometer should be comparable to the resolution setting of the beamline.

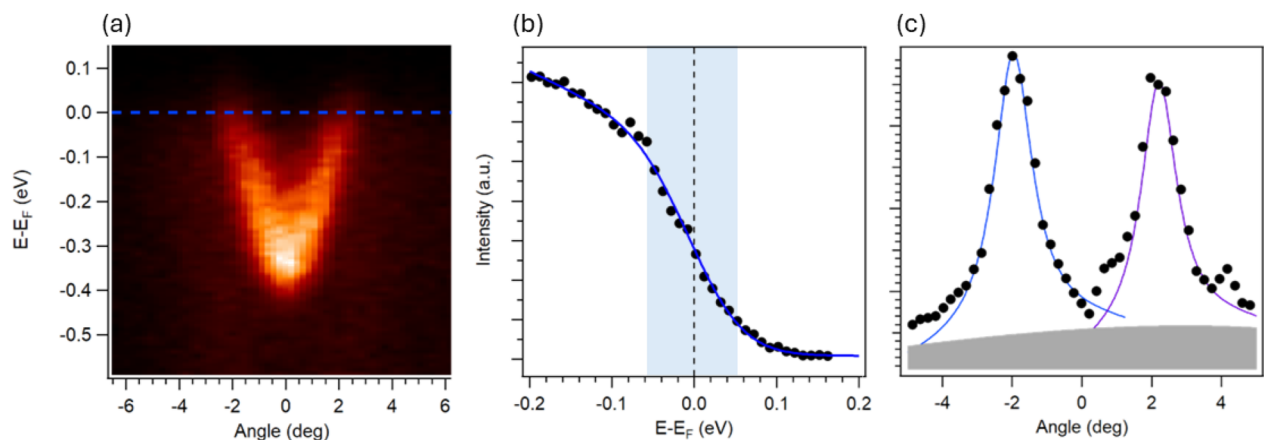


FIG. 8. Experimental resolution determined by the Shockley surface state of Cu(111): (a) ARPES band map recorded at a photon energy of 70 eV and room temperature (300 K). (b) Energy distribution curve (EDC) near the Fermi wave vector at -2° , averaged over $\pm 1^\circ$. The spectrum is fitted with a Fermi–Dirac function convoluted with a Gaussian of 100 meV FWHM. (c) Momentum distribution curve (MDC) at the Fermi energy, averaged over ± 20 meV. The data are fitted with a linear background and two Lorentzians, each with a FWHM of 1° .

In principle, a narrower spectrometer entrance slit of 0.2 mm is also available, which would reduce the analyzer-limited energy resolution to ~ 25 –30 meV at the same pass energy. However, operating with such a narrow analyzer slit would require closing the beamline exit slit to a comparable resolution to benefit from it, leading to an additional reduction of the photon flux. The overall counting time for the band map displayed in Fig. 8(a) was of the order of 30 min. Taking both effects into account, the total count rate would be reduced by approximately one order of magnitude compared to the 0.5 mm slit setting, resulting in significantly longer acquisition times. Under near-ambient-pressure conditions with even higher attenuation (factor 2–10, depending on gas and pressure), this loss in throughput is, therefore, considered impractical for most cases.

The momentum resolution is evaluated from the momentum distribution curve (MDC) at the Fermi energy (± 20 meV), as shown in Fig. 8(c). The MDC was fitted with a quadratic background and two Lorentzian peaks corresponding to the two branches of the Shockley surface state. Each peak exhibits an FWHM of 1° , which closely reflects the angular resolution of the electron-optical system, as the intrinsic width is here about negligible, cf. the results from LASER ARPES.²³

In summary, the achieved energy and angular resolution are fully acceptable for NAP-ARPES measurements and are consistent with the intended operating regime of the instrument. The resolution represents a balanced compromise between spectral performance and transmission, which is essential for measurements under near-ambient-pressure and operando conditions. These results confirm that the spectrometer provides reliable momentum-resolved information while maintaining sufficient count rates for practical NAP-ARPES experiments.

V. APPLICATIONS

A. Graphite and argon gas

This first test with highly oriented pyrolytic graphite (HOPG) was part of the commissioning of the NAP-XPS endstation after the lens upgrade and confirmed the setup for low-energy

angular-resolved photoemission under near-ambient conditions. Although HOPG was chosen for its simplicity and well-characterized electronic structure, it is not without scientific interest: HOPG serves as a model system for layered materials, provides insights into π -band dispersion near the Dirac point, and offers a benchmark for studying gas adsorption and interfacial charge transfer. The scientific case will become significantly more compelling when catalytic surfaces or reactive interfaces are introduced, enabling real-time observation of electronic structure changes during chemical processes.

HOPG chunks were cleaved under UHV with Scotch tape and measured at room temperature (RT). Figure 9 shows ARPES spectra of graphite (HOPG) near the K-point recorded at different photon energies, both in vacuum and in the presence of 1 mbar of argon. The introduction of argon produces distinct atomic emission lines in the spectra, as highlighted in the energy distribution curve on the right, where the Ar 3s and 3p excitations are visible. While this measurement primarily serves as a proof of concept for near-ambient pressure ARPES (NAP-ARPES), it demonstrates the feasibility of performing angle-resolved studies under gas-phase conditions.

B. Zinc oxide and hydrogen gas

As the next test case for NAP-ARPES, the band structure of the ZnO(10-10) surface was measured under hydrogen pressure using soft x rays (439 eV) at RT. The spectra are displayed in Fig. 10 ($w = 0.5$ mm, $E_p = 100$ eV, counting time 30 min). The clean surface was prepared by one cycle of Ar ion sputtering [$p(\text{Ar}) = 1 \times 10^{-5}$ mbar, $U = 1000$ V, $I(\text{ion}) = 10$ mA, 20 min] and annealing (900 K, 10 min) and afterward confirmed by LEED and XPS, showing well-defined band dispersion consistent with previous studies.²⁸

Upon increasing the hydrogen pressure up to 1 mbar, no significant changes in the band structure are observed, in particular, no indication of surface metallization or band bending. This demonstrates that the limiting factor is the applied pressure and activation conditions: under these conditions, molecular hydrogen does not dissociate efficiently on the ZnO surface. This is consistent with previous work,²⁴ observing surface metallization only when atomic

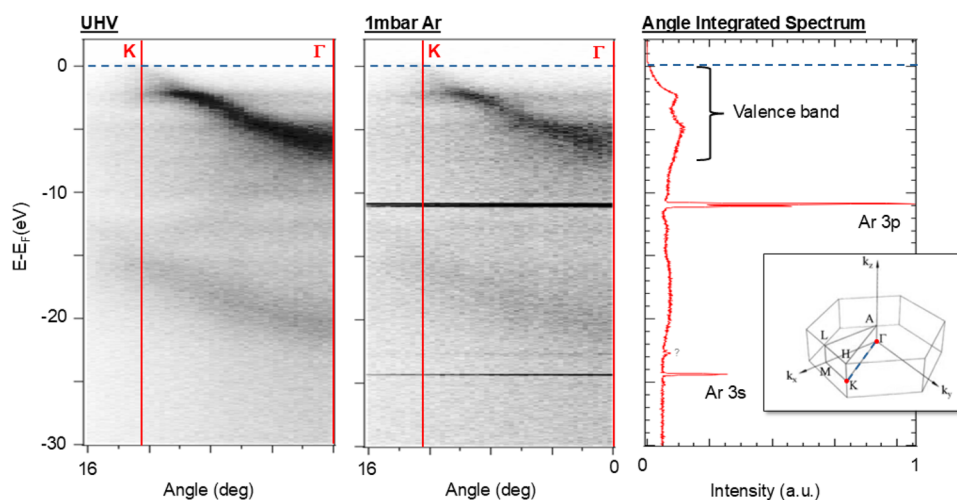


FIG. 9. ARPES spectra of graphite (HOPG) measured along the Γ -K direction in vacuum and under 1 mbar of argon at room temperature with a photon energy of 100 eV, $w = 0.5$ mm, $E_p = 20$ eV, and an overall instrumental energy resolution of ~ 100 meV (beamline + analyzer). Each spectrum was acquired within 20 min of counting time. The characteristic band structure remains well resolved even at elevated pressure. The presence of argon introduces additional atomic emission lines in the spectra, as highlighted in the energy-distribution curve on the right, where the Ar 3s and Ar 3p excitations are clearly visible.

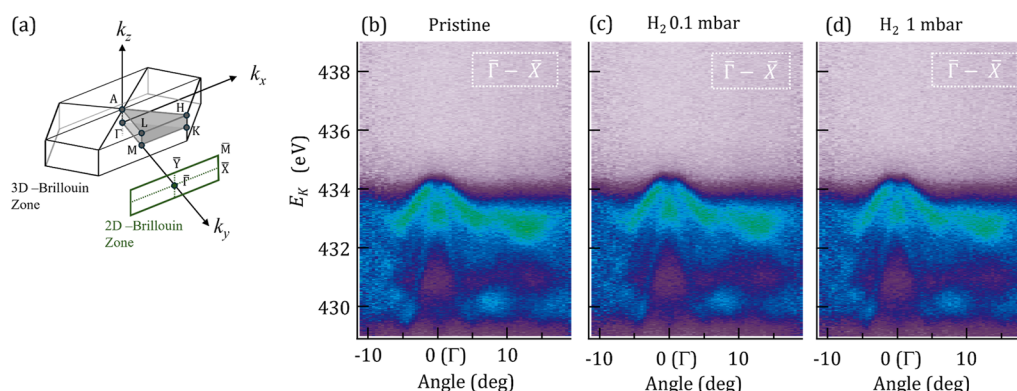


FIG. 10. ARPES spectra of ZnO(10-10) near the Γ -point with and without hydrogen gas up to 1 mbar. (a) The 3D Brillouin zone of ZnO with the projected 2D Brillouin zone of the Zn(10-10) surface. (b) Intensity plot of the ARPES spectra of the pristine ZnO(10-10) surface cut along k_x in the Γ -M-K plane. (c) and (d) Intensity plots of the ARPES spectra with 0.1 mbar of hydrogen gas and 1 mbar of hydrogen gas introduced. Note that here the energy axis is displayed as kinetic energy (rather than $E-E_F$) due to charging-induced uncertainty in the Fermi-level position of semiconducting ZnO. Measurements were performed at room temperature using $h\nu = 439$ eV, analyzer slit width $w = 0.5$ mm, pass energy $E_p = 100$ eV, and an overall energy resolution of ~ 250 meV.

hydrogen was supplied via the hydrogen cracking technique using a hot filament. In contrast, for the measurements here (without hydrogen activation by a cracker cell), the present pressure range is insufficient to produce a comparable level of dissociation and surface coverage. This also indicates that the OH species on ZnO(10-10), observed under a hydrogen pressure of 0.3 mbar, is not highly ordered enough to produce the surface band changes.²⁵ The underlying reason is the high activation barrier for H_2 dissociation, which requires either atomic hydrogen sources or enhanced reaction rates.

These results show that hydrogen-induced changes in the electronic structure cannot be achieved under the present conditions, as higher pressures (above ~ 10 mbar) would be required; however, at such pressures, signal attenuation severely limits the achievable count rate, and more improvement may be required. At the same

time, the measurements clearly demonstrate that soft x-ray NAP-ARPES is fully feasible and yields high-quality band structure data under near-ambient conditions.

C. Copper (111) surface and argon gas

The band structures of Cu(111) are measured at RT for performance tests of ambient pressure ARPES. As shown in Fig. 11(a), the well-known surface states of Cu(111) can be clearly resolved right below the Fermi level under UHV conditions.^{23,26,27} The observation of surface states demonstrates the good resolving capability of electron analyzers with high sensitivity. In addition, the sharp band dispersion features coming from the Cu d -band are seen near 2–5 eV binding energy.

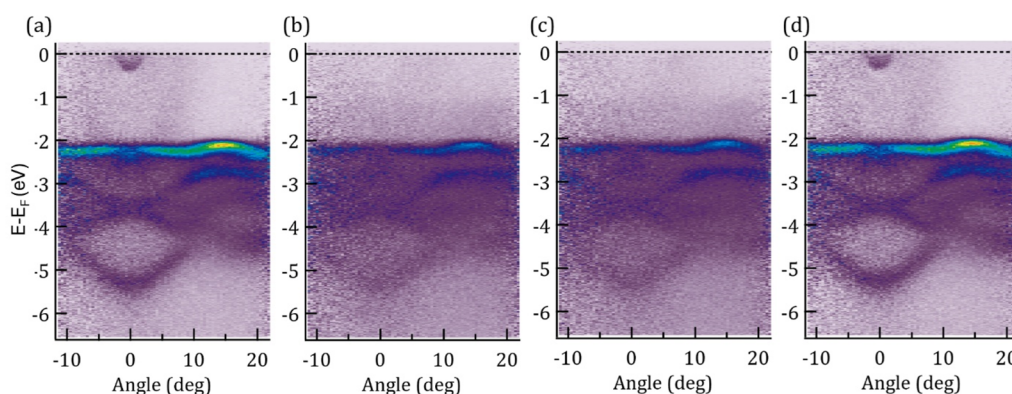


FIG. 11. ARPES spectra of Cu(111) measured near the Γ -point in UHV and under 0.1 mbar of Ar at room temperature using $h\nu = 70$ eV, analyzer slit width $w = 0.5$ mm, pass energy $E_p = 20$ eV, and an overall energy resolution of ~ 100 meV. Panel (a) shows the pristine Cu(111) band dispersion along the Γ -M direction, with the characteristic Shockley surface state clearly visible. Upon introducing 0.1 mbar of Ar, panel (b) shows that the Shockley surface state disappears, while the underlying bulk-like band structure remains well resolved. After pumping out the argon, panel (c) displays only partial recovery of the surface state. Full restoration is achieved after annealing the Ar-exposed sample at 600 K in UHV, as shown in panel (d).

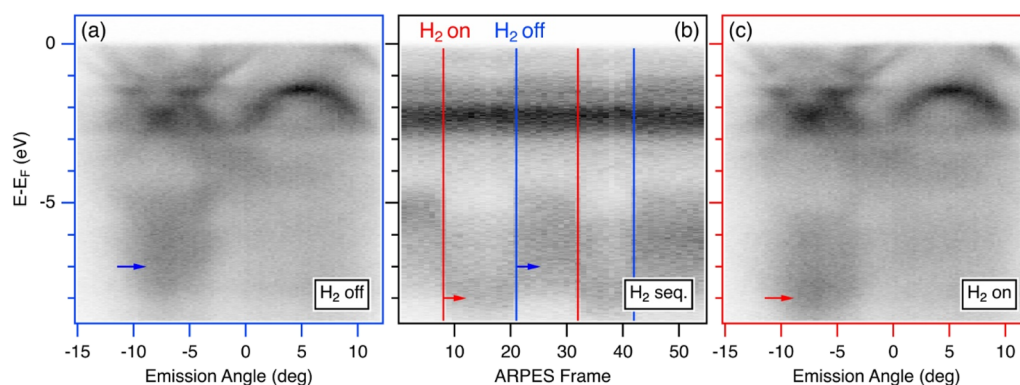


FIG. 12. ARPES spectra of Ru(0001) measured along the Γ -K direction without hydrogen (a) and under 1 mbar of H_2 (c). The time-evolution map shown in (b) highlights the effect of hydrogen exposure: hydrogenation shifts the sections of the deeper Ru 4sp valence band toward higher binding energy (arrows), while electronic states near the Fermi level remain largely unaffected. Measurements were performed at RT using $h\nu = 107$ eV, analyzer slit width $w = 0.5$ mm, pass energy $E_p = 20$ eV, and an overall instrumental energy resolution of ~ 100 meV.

When Ar gas is introduced, the observed surface state immediately disappears, as shown in Fig. 11(b). The non-dispersive features of Ar gas exist at higher binding energies, which are not shown in Fig. 11. When the Ar gas is pumped out, the band structure is almost identical to that of the Cu surface with Ar gas exposure, as shown in Fig. 11(c). When the Cu is later annealed at 600 K under UHV and then measured at RT, the initial band structures with the surface state are fully recovered, consistent with the removal of weakly bound species.

Overall, we may attribute the observed behavior to a residual oxygen impurity in the Ar gas line, which was confirmed later with core-level XPS; however, the relatively low recovery temperature (600 K) suggests that strong chemisorption alone may not fully account for the effect. Instead, the suppression of the Shockley surface state likely reflects its high sensitivity to the surface potential, where even weak adsorption or subtle modifications of the surface barrier can significantly reduce its spectral weight or coherence. The overall band structures under Ar pressure exhibit significant changes, which are not expected for chemically inert Ar gas, and indicate the influence of the gas environment. However, further systematic studies are required to fully clarify the underlying mechanism.

While the results in Fig. 11 demonstrate the high performance of the NAP-ARPES endstation, they also highlight the critical importance of a clean gas supply. In contrast to conventional XPS, NAP-ARPES is particularly sensitive to even trace contaminants, as subtle changes in the surface potential can strongly affect delicate features such as the Shockley surface state.

D. Ru(0001) and hydrogen gas

Finally, we study the hydrogenation of Ru(0001) by monitoring its band structure under hydrogen exposure. After repeated cycles of Ar ion sputtering [$p(\text{Ar}) = 4 \times 10^{-7}$ mbar, $U = 1000$ V, $I_{\text{ion}} = 10$ μA , 30 min] and flash annealing (1800 K, 3 s) to obtain a clean, unreconstructed surface, the sample was transferred into the NAP-ARPES system under UHV, and the characteristic band structure

was recorded at 107 eV ($w = 0.5$ mm and $E_p = 20$ eV, counting time roughly 10 min per frame) at RT, as shown in Fig. 12(a).

After roughly eight sequential ARPES frames in UHV, introducing 1 mbar of H_2 triggers rapid hydrogenation of Ru(0001) [Fig. 12(b)], producing a pronounced ~ 1 eV shift (arrows) in the well-known high-binding-energy Ru sp-derived valence band, while changes in the d-derived valence states remain minor [Fig. 12(c)]. We interpret this behavior in terms of Ru-H sigma bond formation upon hydrogenation. Upon evacuating the hydrogen after 21 ARPES frames, the hydrogen desorbs again, and the original, unhydrogenated band structure reappears immediately. As Fig. 12(b) shows, this hydrogenation-dehydrogenation process is fully reversible and can be repeated multiple times without noticeable degradation of the Ru(0001) surface quality.

VI. DISCUSSION AND PERSPECTIVE

This work demonstrates that angle-resolved photoemission spectroscopy can be performed under near-ambient pressure conditions at the TEMPO beamline, providing a bridge between conventional UHV-based ARPES and operando surface science. By enabling momentum-resolved measurements during gas exposure, the setup opens new opportunities for studying surface processes under conditions closer to realistic environments.

Our primary experiments confirm the feasibility of this approach. Graphite spectra near the K-point were recorded under vacuum and with 1 mbar argon, showing clear band dispersion and argon-induced atomic emission lines, with the band dispersion remaining unaffected by the argon atmosphere. Cu(111) measurements resolved the Shockley surface state under UHV and revealed its disappearance under argon exposure, emphasizing the sensitivity of the technique to surface chemistry and the importance of clean gas handling. Future developments will, therefore, focus on cleaner gas delivery through shorter and bakeable gas lines, larger line diameters to facilitate bake-out procedures, and the implementation of additional purifier cartridges and cryogenic traps where appropriate. On Ru(0001), reversible hydrogenation was tracked through

shifts in the Ru 4s-derived valence band, illustrating the potential for operando studies of catalytic surfaces. ZnO(10-10) measurements under hydrogen exposure showed stable band structures, confirming the capability to probe semiconductors under gas-phase conditions. These results establish a foundation for future studies on catalytic interfaces, energy materials, and two-dimensional systems. As a forward-looking example, topological insulators have been proposed as catalytic platforms,^{29,30} exploiting spin-polarized surface states to enhance reaction pathways and selectivity. Probing these topological surface states under reaction conditions using NAP-ARPES would provide a direct test of this hypothesis and yield deeper insights.

Despite our significant progress in NAP-ARPES methodology, fundamental constraints remain—the limits of the method need to be considered. The current pressure limit, typically up to about 10 mbar depending on the gas, restricts the range of reactions and materials that can be investigated. Furthermore, unlike UHV-ARPES, NAP measurements cannot typically be performed at cryogenic temperatures, as cooling under gas exposure risks condensation or freezing on the sample surface. This necessitates operation near or above room temperature, which introduces significant phonon activity. Phonon-assisted transitions can disrupt momentum conservation, leading to a gradual loss of band structure resolution, a transition toward the so-called XPS limit, as discussed in Ref. 31. The onset of this effect depends on the material's Debye temperature and the photon energy used; lighter elements and higher photon energies are less favorable for preserving momentum resolution. Nevertheless, high-energy ARPES studies have demonstrated that meaningful band structure information can still be obtained under extreme conditions, even for buried or bulk states (see Refs. 32 and 33). In addition, our results on graphite confirm that meaningful band structure information can still be obtained for a light element at room temperature. However, this depends on the individual compound and all the details.

Our NAP-ARPES functionality builds upon the proven NAP-XPS setup of the Sorbonne Université located at TEMPO. The recent lens redesign has also improved electron transmission for NAP-XPS, which benefits the overall performance of the endstation and indirectly supports NAP-ARPES by ensuring higher signal quality under near-ambient conditions. One of the strengths of the soft x-ray beamline TEMPO is its large photon energy range from 50 to 1500 eV, which allows NAP-XPS, NAP-NEXAFS, and NAP-ARPES to be performed on the same sample under the same experimental conditions. This versatility is particularly valuable for correlating chemical and electronic structure information. In a broader perspective, this development positions NAP-ARPES as a complementary tool to NAP-XPS and NAP-NEXAFS, offering momentum-resolved insights into surface chemistry.

Further improvements to our setup are envisioned to enhance the versatility and precision of NAP-ARPES. An increased automation of the sample manipulator and a transition from the current 5-axis to a 6-axis design would enable comprehensive, larger Brillouin-zone mapping and facilitate complex experimental geometries. In this context, the implementation of deflector-based electron optics would be particularly beneficial for orbital tomography. Other improvements are a cleaner and more flexible gas-handling system. Additional optimization of the analyzer (lens tables and nozzle

design) may help extend the accessible angular range, improving coverage of reciprocal space.

Looking ahead, SOLEIL is accelerating toward its SOLEIL II upgrade,³⁴ which will transform the facility into a fourth-generation diffraction-limited synchrotron. This upgrade is projected to deliver a much smaller beam diameter at TEMPO II and increase photon flux by a factor of two to three. This will be very beneficial for NAP-ARPES, enhancing the maximum pressure usable and the energy- and momentum-resolutions. In addition, the photon energy range of TEMPO will be extended up to 2500 eV, significantly benefiting NAP-XPS and, indirectly, NAP-ARPES by enabling deeper core-level studies and improved chemical sensitivity under operando conditions.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Lenart Dudy: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Elisa Auf-fray:** Investigation (equal). **Jean-Jacques Gallet:** Conceptualization (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Writing – original draft (equal). **Fabrice Bournel:** Conceptualization (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Writing – original draft (equal). **Meryem Bouaziz:** Investigation (equal). **Bongjin Simon Mun:** Conceptualization (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Resources (equal); Validation

(equal); Writing – original draft (equal). **Subin Jang**: Investigation (equal). **Yuki Tsujikawa**: Data curation (equal); Investigation (equal); Software (equal). **Hiroshi Kondoh**: Investigation (equal). **Valentin Mischke**: Investigation (equal). **Philipp Käßler**: Investigation (equal). **Vedran Jovic**: Conceptualization (equal); Investigation (equal); Methodology (equal). **Simon Moser**: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Validation (equal); Writing – original draft (equal). **Sven Maehl**: Conceptualization (equal); Methodology (equal); Project administration (equal); Resources (equal); Validation (equal); Writing – original draft (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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