Supporting Information:

Stable mass-selected AuTiO_x nanoparticles for CO oxidation

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S1 HRTEM images of AuTiO_x nanoparticles

The HRTEM image contrast pattern of the AuTiO_x nanoparticles was studied through an image focal series, in which consecutive HRTEM images of the nanoparticles were captured at various defocus (Δf) values (**Figures S1a-d**). The images are displayed with defocus from $\Delta f = -680$ nm to $|\Delta f| < 30$ nm. Δf was estimated by calculating the Fast Fourier Transforms (FFTs) of the images (**Figures S1e-h**) and by fitting the contrast reversals of the resulting concentric ring patterns with the HRTEM contrast transfer function (CTF) (D. B. Williams and C. B. Carter, "Transmission Electron Microscopy: A Textbook for Materials Science," 2nd Edition, Springer, New York, 2009, pp. 1-757.):

$$CTF(\boldsymbol{g}) = \sin\left(\pi\lambda\Delta f|\boldsymbol{g}|^2 + \frac{1}{2}\pi C_s\lambda^3|\boldsymbol{g}|^4\right)$$

where λ is the electron wavelength, g is the 2D spatial frequency vector and C_S is the spherical aberration.

The projections of **Figures S1a-d** display 7 dark circular features of ca. 2 nm diameter accompanied by a brighter contrast rim surrounding each of them. As Δf is varied the contrast of these features change from being most pronounced at the largest $|\Delta f|$ values (**Figures S1a-b**) and to almost vanish as $|\Delta f|$ is minimized (**Figures S1c-d**).



Figure S1 Effect of defocus on HRTEM images of AuTiO_x nanoparticles. a-d) HRTEM images of AuTiO_x nanoparticles at various defocus (Δf). e-h) FFTs of the images displayed in a-d. Image pixel size: 0.037 nm/pixel.

Increasing $|\Delta f|$ increases the contrast of larger feature sizes, but it also increases feature blurring due to contrast delocalization ($|\Delta R|$) which is given as (D. B. Williams and C. B. Carter, "Transmission Electron Microscopy: A Textbook for Materials Science," 2nd Edition, Springer, New York, 2009, pp. 1-757.):

$$\Delta R(\boldsymbol{g}) = \lambda \boldsymbol{g} \left(\Delta f + C_S \lambda^2 \boldsymbol{g}^2 \right)$$

The applied HRTEM imaging conditions are characterized Cs = -10 μ m, λ = 1.97 pm (300 keV), resulting in a contrast delocalization of a feature sized 2 nm (g = 0.5 1/nm) of:

$$\Delta R \left(C_S = -10 \ \mu\text{m}, \lambda = 1.97 \ \text{pm}, g = 0.5 \frac{1}{\text{nm}} \right) = 10^{-3} \left(\Delta f - 0.01 \ \text{nm} \right)$$

Hence a 2 nm wide feature is blurred by $\cong \Delta f/1000$ and amounts to ~ 1 Å for $\Delta f \cong 100$ nm.

Furthermore, **Figure S2** shows an analysis of the $|\Delta f|$ dependency of the bright rim's width. The width is estimated from a single location for one of the nanoparticle projections and indicated by the superimposed lines in **Figure S2a-c**. **Figure S2d** shows that the estimated rim width shortens as the magnitude of Δf decreases. Based on linear regression, the intercept at $\Delta f = 0$ gives a rim width of 0.8 Å. Hence, despite the bright rim being invisible due to contrast suppression at zero defocus, the present analysis shows the bright rim is a physical feature of width 0.8 Å that increases at larger defocus due to delocalization.



Figure S2 AuTiO_x rim feature dependency on Δf in HRTEM. a)-c) HRTEM images of AuTiO_x nanoparticles acquired at various Δf , with annotations showing estimated rim feature width. d) Estimated rim width vs. Δf as well as linear regression of the data points. Image pixel size: 0.037 nm/pixel.

To further support the hypothesis that this feature is not just an imaging artefact but a physical feature of the AuTiO_x nanoparticles, **Figure S3** shows a HRTEM image of Au nanoparticles acquired at a high defocus of $\Delta f = -310$ nm (as evidenced by its corresponding FFT). and the absence of such a bright rim feature indicated that it is an inherent feature for the AuTiO_x nanoparticles.



Figure S3 HRTEM image of Au nanoparticles. a) HRTEM image of the nanoparticles. b) FFT of a). Image pixel size: 0.036 nm/pixel.

Lastly, a near-zero defocus image of an AuTiO_x nanoparticle was acquired in a high-order zone axis orientation (**Figure S4a**). As near-zero defocus suppresses low spatial frequencies, both the bright contrast rims and the darker circular projected core for $AuTiO_x$ nanoparticles are associated with reduced contrast. Instead, contrast of high spatial frequencies remains and reflects the crystal lattice fringes of the $AuTiO_x$ nanoparticle core. These lattice fringes correspond to crystal lattice planes and spacings closely matching FCC Au in the [011] zone axis (**Figure S4b**). This suggests that the darker circular projections of the $AuTiO_x$ nanoparticles mainly consists of structured FCC Au and that the Ti are more abundant in the brighter rim projections. This is also consistent with the observation that the round Au nanoparticle projections (**Figure S3**) have a similar contrast to the darker circular feature of the $AuTiO_x$ nanoparticles. Furthermore, the contrast difference between the core (darker contrast) consisting of a high abundance of Au and the outer rim (brighter contrast) consisting of a higher abundance of lighter elements such as Ti and O is also as expected for a HRTEM image.



Figure S4 HRTEM image of a AuTiO_x nanoparticle. a) HRTEM image demonstrating visible core and transparent shell of an AuTiO_x nanoparticle. Core displays lattice fringes matching Au FCC observed along the [011] zone axis. b) The FFT of a) used to assign the nanoparticle core to the Au FCC projection based on crystal structure obtained from ICSD-52249 (ICSD release 2023.2) (Professor

E.A. Owen M.A. D.Sc. & E.L. Yates M.Sc. (1933) XLI. Precision measurements of crystal parameters

, The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 15:98, 472-488, DOI: 10.1080/14786443309462199).

 $|\Delta f| < 25$ nm. Image has been rebinned by 2, from pixel size 0.011 nm to 0.022 nm. DR = 55 e⁻/(Å² s).

S2 AuTiO_x and Au diameter measurements

To estimate a projected mean core size for the AuTiO_x nanoparticles two HRTEM images containing the nanoparticles were analyzed as displayed in **Figure S5**. Due to the approximate circular shape of the projections, their diameter was estimated by a 1-dimensional length measurement along an arbitrary diameter axis. The length measurements start and end at opposite sides of the circular projections as indicated by the line annotations of **Figure S5**. Using this methodology, a mean and standard deviation of the projected diameter of the 28 nanoparticle cores of **Figure S5** were estimated to be 2.1 nm and 0.2 nm, respectively. An elongated AuTiO_x nanoparticle was observed for the lower right part of image **Figure S5a**. As this nanoparticle was observed to be an outlier in its shape and size it was excluded from the core-size estimation. This nanoparticle appears to have double the size of the other present nanoparticles, which could be due to an agglomeration of 2 nanoparticles but can also be explained by a non-zero deposition current of double-mass nanoparticles in the cluster source.



Figure S5 Two HRTEM images used for $AuTiO_x$ nanoparticle core-size measurements a)-b). The superimposed diameters reflect the core-size distribution. Images were acquired under room temperature and 10^{-6} mbar conditions on sample after synthesis and insertion into the electron microscope. Image pixel sizes: 0.037 nm/pixel and 0.017 nm/pixel respectively.

The mean diameter size of the Au nanoparticles was estimated in a similar manner to the core of the AuTiO_x nanoparticles. Like the AuTiO_x core, the projections of the Au nanoparticles are observed to be dark and circular as observed in section S1. **Figure S6** shows the diameter of 19 nanoparticles included in the analysis and the mean and standard deviation of the projected diameter were estimated to be 2.1 nm and 0.2 nm, respectively.



Figure S6 HRTEM image used for Au nanoparticle size measurements. The superimposed diameters reflect the Au nanoparticle size distribution. Images were acquired under room temperature and 10⁻⁶ mbar conditions on a sample after synthesis and insertion into the electron microscope. Image pixel size: 0.036 nm/pixel.

For the images of **Figure S5a**, **S5b** and **Figure S6** the defocus of the HRTEM images were measured to be \sim -180 nm, -220 nm and -250 nm in their order of appearance. As the corresponding contrast delocalization is on the order of a few Å, for a 2 nm feature size which means that the contrast delocalization is on the order of the nanoparticle collection's core diameter standard deviation.

S3 Elemental mapping by EDS

AuTiO_x nanoparticles of size 5.5 nm were deposited by the cluster source on a lacey carbon Cu grid and transferred through ambient to an FEI Titan Analytical 80-300 ST transmission electron microscope equipped with a pre-objective lens spherical aberration corrector. The microscope was operated at a primary electron energy of 300 keV in scanning transmission electron microscopy (STEM) mode with simultaneous high-annular dark field (HAADF) detection for imaging and Energy Dispersive Spectroscopy (EDS) (**Figure S7**).



Figure S7 Combined imaging and spectroscopy of AuTiO_x nanoparticles. a) HAADF-STEM image of 5.5 nm AuTiO_x nanoparticles on lacey carbon. b) EDS map of Au and Ti distributions superimposed on the HAADF-STEM image in a). c) EDS linescan across an AuTi nanoparticle of diameter 5.5 nm showing the profiles of Ti and Au.

Figure S7a shows the HAADF-STEM image of the 5.5 nm nanoparticles, and **Figure S7b** shows the simultaneous Au and Ti distributions determined by EDS. **Figure S7c** indicates that Ti originates from a larger area than Au. Au is mostly concentrated near the center of the particle, and the Au/Ti ratio decays further towards the edges of the particle.

S4 XPS data analysis for the AuTiO_x nanoparticles on SiO₂

The AuTiO_x nanoparticles deposited on a SiO₂-coated microreactor were measured in XPS in a separate UHV chamber, *i.e.*, after the chip had been removed from the cluster source and exposed to air. This caused the oxidation of the outer shell. **Figure S8a** shows the full survey spectrum of the SiO₂ chip with the AuTiO_x nanoparticles (5% coverage). Signals from the nanoparticles (Au and Ti) and the support (Si and O) are observed, as well as some trace contaminants.



Figure S8a XPS data survey scan of the $SiO_2 + AuTiO_x$ nanoparticles sample using a monochromatic Al K α X-ray source (1486.68 eV). Data was taken after the sample had been transferred in air. Trace amounts of F, as well as C and N were present in addition to the signals from Si, O, Au and Ti.

The Ti and Au peaks which are also shown in **Figure 3** in the manuscript were fitted to obtain the At% ratio. The data was fitted and analyzed using CasaXPS. The data was first smoothed using linear smoothing width 3, and the energy axis was calibrated to the C 1s peak for adventitious carbon at 284.8 eV. Subsequently, the peaks were fitted using a Shirley background, and individual sub peaks were fitted with position constraints according to reference values from¹. The At% (percentage atomic concentrations) were calculated using the total area of each peak and including the influence of the R.S.F. factors for each peak component (Ti 2p 1/2: 2.59, Ti 2p 3/2: 5.22, Au 4f 5/2: 7.54, Au 4f 7/2:

¹ J. F. Moulder, W. F. (1992). Handbook of X-ray Photoelectron Spectroscopy. Perkin-Elmer Corporation.

9.58). The boundaries of the fittings were varied manually to estimate the accuracy of the fitting, which induced changes in the resulting output of 1-2 At% away from the 38/62 At% ratio stated. To understand the observations in greater detail, the intensity of the signal and probing depth in XPS for the core-shell nanoparticles must be considered.

The intensity of the detected signal in XPS follows the relation $I = I_0 e^{-x/\lambda}$, where I_0 is the initial intensity, which decays to 37% of its value at $x = \lambda$, the mean free path of the electrons in a given material. According to the universal curve, λ of electrons in e.g. Au, with kinetic energy ~ 1400eV (such as those detected for the 4f level in this study), is ~ 2nm². With this value for the mean free path, the signal intensity in XPS behaves as demonstrated in the figure below.

Calculating the expected Au/Ti signal based on a spherical model is not analytically straightforward, but to simplify the problem, the nanoparticle can be approximated as a larger cylinder with a smaller cylinder inside made of Au as shown in orange below. By matching the volume of the cylinders to the spherical particle, effective radii of the cylinders can be inferred, and the integral can be performed in the vertical axis through the shell – core – shell structure, where the height h is estimated from the probing depth through the nanoparticle. That way, the shielding of the signal through the shell, and the contribution from the core vs shell is estimated as follows:



As shown above, the intensity of the signal decays exponentially through the nanoparticle. If all Au atoms were concentrated in a 2.1nm core of the nanoparticle, then the Au/Ti signal expected would be Au/Ti = 0.25, as shown. Alternatively, the height of the cylinder can be calculated using $h = \frac{V}{\pi r^2} = \frac{4}{3}r$,

² Chorkendorff, I. & Niemantsverdriet, J. W. Concepts of Modern Catalysis and Kinetics (Wiley-VCH Verlag, 2003)

where the radius of the cylinder is chosen to match that of the sphere, in which case the answer is similar - Au/Ti = 0.26. It is also worth noting that varying the value of λ between 1.5 - 2.5 nm causes only a minor change in the obtained value of Au/Ti, of \pm 0.02. Therefore, the detected ratio of 38/62 suggests that more Au is present in the shell of the particle than the Au present in the core. If the Au atoms were uniformly dispersed throughout the nanoparticle, the Au/Ti signal expected would be 50/50, and therefore the reduced fraction of Au in the detected signal also indicated that the Au is concentrated deeper than in the top layers of the nanoparticle.

S5 Activity measurements raw data and further analysis



Figure S9 First two temperature ramps for AuTiO_x nanoparticles: MRFR04 (left) and MRFR05 (right). In both experiments, it was necessary to reach T > 220 °C to activate the catalyst.



Figure S10 Arrhenius plot for a) Au and b) $AuTiO_x$ catalyst. The rate of reaction was calculated with the steady state signal at the reported temperatures after catalyst activation. The temperatures were chosen to be far from full conversion and not to be limited by diffusion. Even though for $AuTiO_x$ at those temperature we see a much lower activity for the reasons explained in the main text, the lower activation energy might indicate a better active site for CO oxidation (gold atoms on the TiO₂ surface).



Figure S11 Raw data for the stability measurements on AuTiO_x MRFR05. Ar (M40) was used as control gas for normalizing towards temperature effects and QMS signal fluctuations. These data were collected after the ones represented in **Figure S9**.

Au sample CO₂ production vs temperature ramps



Figure S12 a) Raw data of the activity measurements on Au FRMR01. Ar (M40) was used as control gas for normalizing towards temperature effects and QMS signal fluctuations. The red area corresponds to the pump-down period in the microreactor. b) CO₂ production vs T during ramping up and down showing mild deactivation.

S6 SEM images: size measurements



Figure S13 Particle size distribution image processing of the Au FRMR01 sample after reaction for in ImageJ. The counts below 2.1 nm are indicative of deposited double charged particles or counting errors due to the image resolution.



Figure S14 SEM pictures at different magnifications of the post-reaction Au and AuTiO_x sample. All the images are taken with a through-the-lens secondary electron detector at 5kV.

S7 ISS sputter profile: first scan



Figure S15 ISS spectra at different sputter depths for the depth profiling measurements of the AuTiO_x nanoparticles. The spectrum shown in red is the first ISS spectrum acquired from the sample just after loading into UHV – *i.e.*, before any of the surface contamination due to air exposure has been removed by the gentle He⁺ sputtering of the surface. As the spectrum shows, the Au, Ti and O signals are not distinguishable at this stage. Therefore, the 10th cycle was chosen as the first cycle to include in the plot, since here, the background first started being more comparable to the background of the sample before it was originally removed from UHV, and the Au signal is also emerging at this point.

S8 HRTEM measurement plan

The time-temperature profiles of the HRTEM investigations of Au and AuTiO_x nanoparticles are displayed in **Figure S16**. The temperature was ramped up incrementally during the experiment. At each temperature, HRTEM images were acquired of a specific "*primary*" location for the Au and AuTiO_x nanoparticles, respectively and of "*reference*" areas, which were previous to their image acquisition left unexposed to the electron beam during the experiment. The *primary* and *reference* images were compared to differentiate beam-induced and reaction-induced alterations of the samples.



Figure S16 Time-temperature profile for the HRTEM imaging of Au and AuTiO_x nanoparticle samples. As indicated, the samples were exposed to a gas mixture of 2 mbar O_2 and 1 mbar CO.

S9 Beam-induced contamination

For the electron microscopy experiments where the samples were exposed to reactive gasses (as described in section S8), HRTEM images were acquired of a specific "*primary*" location for the Au and AuTiO_x nanoparticles, respectively and of "*reference*" areas, which were previously unexposed to the electron beam in the experiment. In the electron microscope, it was noted from consecutive images of primary areas (see section S10) that darker contrast patches appeared during exposure to 2 mbar CO and 1 mbar O₂, as also displayed in **Figure S17**. These patches formed on the support in-between the AuTiO_x nanoparticles. Moreover, the bright contrast rim around the AuTiO_x nanoparticles also appeared to grow in width. Similar features were absent on the reference areas suggesting they are derived from contamination induced by the electron beam.

The contamination was characterized further by electron energy loss (EEL) spectroscopy. **Figures S18-S19** show EEL spectra acquired of a primary (contaminated) area and a reference area (without previous exposure to the electron beam). The EEL spectra were acquired after the experiment in the high vacuum of the microscope and with the sample at room temperature. The EEL spectra clearly show the presence of a C K edge and a Ni L2,3 edge in the primary area and the absence hereof in the reference area. These deposits could originate from Ni carbonyls in the CO gas. The contamination is further discussed in section S10.



Figure S17 Beam-induced contamination of $AuTiO_x$ nanoparticles. Left) Image before gas insertion. Right) Image immediately after gas insertion. Images were acquired at room temperature prior and post gas exposure, prior to temperature ramp (**Figure S16**). Dose rates for the images: DR = 50 e⁻/(Å² s) and DR = 40 e⁻/(Å² s). Acquired Images have been 2x rebinned, from pixel size 0.037 nm to 0.074 nm.



Figure S18 EEL spectra of a primary and reference area on the AuTiO_x nanoparticle sample. The spectra were obtained with parallel illumination of the sample over a 5 μm wide area with the projection optics operated in diffraction mode with camera length of 195 mm (approximately as this calibration is given by the microscope). The Gatan Image Filter used for EEL spectrum acquisition was operated with entrance aperture diameter 2 mm, energy dispersion 0.2 eV/channel, and exposure of 5 s. The energy offsets between the spectra were aligned by visual inspection using the nitrogen K edge peak.



Figure S19 EELS spectra comparing contaminated and non-contaminated areas, in the oxygen to nickel core loss region. Same acquisition and post-processing procedure performed as done for the data of Figure S18.

S10 Complementary observations of Au and AuTiO_x nanoparticles

Figure S20 shows complementary HRTEM images of a primary area of AuTiO_x nanoparticles acquired consecutively during exposure to the reactive gas environment. With increasing temperature (and time), the images show darker spots on the supporting material and an increase in the width of the bright contrast rim. This beam-related contamination is the same as that documented in section S9. These changes differ from the similar observations of the reference area (**Figure 7**) and are thus indicative of a beam-induced sample alteration. Moreover, the AuTiO_x nanoparticles are observed to maintain their start positions during gas and temperature observations.



Figure S20 HRTEM images of a primary area of the $AuTiO_x$ sample during exposure to 2 mbar CO and 1 mbar O_2 at elevated temperatures. The images are cropped from originals and represents a pixel size of 0.037 nm/pixel.

Figure S21 shows HRTEM images acquired of a primary area of the Au nanoparticle sample during exposure to the reactive gas environment. The images reveal no indications of contamination as observed for the AuTiO_x nanoparticle sample (**Figure S20**). Regarding the difference in carbon and nickel accumulation, it is likely the gas bypassed the activated carbon filter for carbonyl decomposition on the microscope's gas handling system in the AuTiO_x nanoparticle experiment. However, we note the absence of these contaminants in the reference areas of AuTiO_x and therefore the manuscript focuses on these observations. However, the Au nanoparticles develop tracks similar to those in **Figure 7**.



Figure S21 HRTEM of a primary area of the Au nanoparticle sample during exposure to 2 mbar CO and 1 mbar O₂ at elevated temperatures. The images are cropped from the originals and represent a pixel size of 0.037 nm/pixel.

Figure S22 shows HRTEM images acquired at lower magnification of the Au nanoparticle sample, comparing an area before exposure to the reactive gas environment and elevated temperatures (Figure S22a) and after exposure to the reactive gas environment and elevated temperatures up to 400°C (Figure S22b) (at the end of the temperature ramping of Figure S16). The images show that nearly all nanoparticles are displaced and have formed a track on the adjacent support. Noticeably, Au nanoparticles protrude from the edge of the silicon nitride support into vacuum. As these Au nanoparticles also are associated with a brighter track, it is likely that all tracks similarly represent a filament growth occurring between the Au nanoparticles and the support.



Figure S22 HRTEM image at low magnification of the Au nanoparticle sample. a) Image acquired at room temperature with exposure to 1 mbar CO and 2 mbar O₂. b) HRTEM image acquired at same area as a) at room temperature after the heating procedure in **Figure S16** and subsequent removal of CO and O₂ from the microscope gas cell. Image pixel size: 0.093 nm/pixel.

Figure S23 shows HRTEM images of the Au nanoparticles and the tracks formed during exposure to the reactive gas environment. The images reveal crystal lattice fringes in the tracks (**Figures S23b-c**). FFTs of the cropped areas 1-3 in **Figures S23b-c** reveal the corresponding lattice spacings of 2.4 Å, 2.1 Å and 1.3 Å. As a great number of crystalline materials have lattice fringes corresponding to these length scales, use of supplementary localized TEM EEL spectroscopy of the filaments would be beneficial to further characterize them.



Figure S23 HRTEM images of the tracks formed at the Au nanoparticle. a) HRTEM image showing an ensemble of Au nanoparticles. Image pixel size: 0.036 nm/pixel. b)-c) Close-up HRTEM images of 3 specific nanoparticles. Image pixel size: 0.017 nm/pixel. The square outlined areas are used for the FFTs in d)-f). HRTEM images cropped from original images.

S11 Microreactor setup schematics



Figure S24 Front and back view of the microreactors used for all the catalytic activity experiments. The central reactive area is 3 μm deep. The total reactor volume (red dotted area) is ~240 nL. Photos by Thomas Pedersen.



Figure S25 Schematic of the cooled anodic bonding setup.

S12 Catalytic activity data: mass spectrometer calibration and further treatment

All the catalytic activity plots were processed with a python script. The raw data were retrieved from a Quadrupole Mass Spectrometer (QMS). To convert the raw current signal in A to moles/seconds, the microreactors and the QMS were calibrated using a baratron.



Figure S26 QMS raw signal of the calibration curves for MRFR04. Blue (CO) and red (O₂) lines are to be read in Amperes (left y axis). The grey curve (baratron pressure) is expressed in mbar on the right axis.

The baratron consists in a known volume connected to the outlet of the microreactor (referred as O2 in **Figure S24**). The reactor was filled with 1 bar of pure CO, O_2 , and CO_2 . Once a stable signal in the QMS was reached, the valve to the mass spectrometer was closed, causing an increase of pressure in the line. The pressure evolution was recorded by the baratron. An example of a typical calibration is shown in **Figure S26**.

The basic concept relies on simple calculations using ideal gas approximations as follows:

$$P \cdot V = n \cdot R \cdot T$$
$$\frac{\Delta P \cdot V}{t} = \frac{\Delta n \cdot R \cdot T}{t}$$
$$\dot{P} \cdot V = \dot{n} \cdot R \cdot T$$

Where: P = baratron pressure (mbar); V = reactor volume (236 nL); n = moles of the gas to calibrate (nmol); R = ideal gas constant (= 83.14 nL·mbar·K⁻¹·nmol⁻¹); T = temperature (K)

The only variables in time in the formulas are P and n. By extrapolating the baratron pressure in the graph at two consecutive time stamps, \dot{P} could be calculated. \dot{n} was derivated as follows:

$$\dot{n} = \frac{\dot{P} \cdot V}{R \cdot T}$$

Once the molar flow \dot{n} was calculated for every gas, the calibration factors were derived by simply dividing the QMS baselined signal at 1 bar with the molar flow:

$$F_M^x = \frac{QMS \ signal}{\dot{n}^x}$$

With $x = CO_2$, CO, O₂, Ar.

The as described concepts were implemented in a python script and complemented with background subtraction.

After the QMS signals were calibrated and translated in nmol/s, the data were further normalized vs Ar (control gas) and Au active surface area (when needed).

The full script is available on the following GitHub link for transparency: <u>https://github.com/filro/QMS-Script_PostProcessing.git</u>