

# A Quantitative Transformer-Augmented and Virtual-Material-Multiplexed Plasmonic Hydrogen Sensor for Chemically Deactivating Humid Air Environments

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## Article

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*A Quantitative Transformer-Augmented and  
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Sensor for Chemically Deactivating Humid Air  
Environments*

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## Abstract

Quantitative gas sensing in realistic, chemically complex environments, such as urban air, remains challenging because interferent species can competitively adsorb, deactivate sensor surfaces and cause cross-sensitivity. This limits many promising sensor technologies, especially where absolute quantification rather than classification is required. Here, we report a waveguide-based nanoplasmonic H<sub>2</sub> sensor comprising seven different physical metal nanoparticle arrays that are optically convolved into 64 virtual sensing materials. Combined with an encoder-only transformer deep-learning model, this architecture enables accurate H<sub>2</sub> quantification in a simulated Jakarta urban-air environment based on real weather data, with high and varying humidity and deactivating CO, CO<sub>2</sub> and NO<sub>x</sub> interferents. The same model also quantifies the interfering species throughout the measurement by actively exploiting cross-sensitivity. Finally, transformer attention maps identify which virtual sensing regions dominate under different sensing conditions, providing a future route to sensor-material optimization using information collected from devices deployed in realistic operating environments.

## Introduction

Sensors are of ever-increasing importance for energy systems, transport, manufacturing and urban infrastructure, where real-time monitoring is essential for reliability and risk management. Yet many new sensor concepts that perform well in the laboratory experience difficulties under real operating conditions because interferences deactivate sensing surfaces, generate cross-sensitivity and cause drift that requires repeated recalibration.<sup>1-5</sup> This problem is especially pronounced in gas sensing, where target analytes are often dilute and must be quantified against fluctuating humidity, temperature and chemically diverse backgrounds that change over time.

Electronic noses<sup>6</sup> seek to solve this challenge by combining partially selective sensors whose collective response is decoded statistically or by machine learning. Such sensor arrays have been realized with metal oxides,<sup>7-10</sup> polymers,<sup>11</sup> carbon nanotubes,<sup>12</sup> quantum dots<sup>13</sup> and nanoparticles,<sup>12,14,15</sup> either as purpose-built devices<sup>8,11,12,14-16</sup> or as assemblies of commercial sensors.<sup>17,18</sup> Although *classification*, i.e., identification of which species are present in the analyzed gas, is now mature in the field of electronic noses,<sup>7,8,10,12-15</sup> absolute *quantification* in realistic gas mixtures remains much less developed. Existing early demonstrations include ppb formaldehyde detection at 90% RH,<sup>16</sup> quantification of CO, H<sub>2</sub>S and NO<sub>2</sub> mixtures,<sup>10</sup> aromatic hydrocarbons with interferences,<sup>11</sup> simultaneous CO, NH<sub>3</sub>, NO<sub>2</sub>, CH<sub>4</sub> and acetone detection,<sup>19</sup> RH and NO<sub>2</sub> field measurements,<sup>20</sup> and outdoor monitoring of NO<sub>2</sub>, SO<sub>2</sub>, CO and volatile organic compounds.<sup>13</sup> However, these studies are limited by relying on single analytes,<sup>16</sup> one-at-a-time exposures<sup>19</sup> or short tests that do not reproduce realistic concentration dynamics.<sup>13</sup> A comparison with representative prior gas-sensing and machine-learning demonstrations is provided in Supplementary Note 4 (**Table S13**).

Important for this state-of-the-art has been the development of methods for the interpretation of the data provided by an array of sensors. Here, linear regression and classification models<sup>21-25</sup> enabled early progress but often simplified the inference problem by discarding structure in the data, thereby reducing robustness when measurement and calibration conditions diverged.<sup>24-26</sup> Deep-learning approaches, including first convolutional and recurrent models, address this by using full transient array responses

instead of steady-state amplitudes or handcrafted descriptors.<sup>4,24,25,27-29</sup> More recently, transformers have become particularly attractive because they capture long-range temporal dependencies and flexible interactions between sensor channels without requiring the problem to be rewritten as a small set of handcrafted rules.<sup>30,31</sup>

One specific gas sensing context in which the above outlined challenges are equally apparent as urgent is hydrogen ( $H_2$ ) sensors since  $H_2$  safety and process monitoring are critical for emerging energy systems.<sup>1,32-34</sup> Here, laboratory sensors have achieved sub-second responses,<sup>35-38</sup> ppb detection limits<sup>35,39,40</sup> and dynamic ranges spanning more than seven orders of magnitude.<sup>37</sup> Translation to practical devices nevertheless remains difficult<sup>1</sup> because most breakthroughs were obtained under idealized conditions, including vacuum,<sup>35,36,38</sup> inert Ar<sup>37</sup> or  $N_2$ ,<sup>35</sup> or clean synthetic air.<sup>39,41</sup> Tests with  $H_2O$ , CO,  $CO_2$ ,  $NO_2$  or NO interferants have mainly assessed selectivity to individual contaminants rather than their impact on the response to  $H_2$ .<sup>41-53</sup> When deactivation by  $H_2O$ <sup>44,45,47,49-51,54</sup> or other contaminants<sup>35,36,38,48,55</sup> has been examined, it has typically involved one contaminant at a time in Ar,  $N_2$ <sup>35,44</sup> or synthetic air.<sup>36,38,45,47-51,54,55</sup> Critically, however, these conditions do not represent typical target operating conditions of a technically relevant  $H_2$  sensor application, i.e., gas mixtures which include a multitude of interfering and potentially deactivating gas species, which by themselves potentially also are interesting for quantitative monitoring.

Here we introduce a virtually material-multiplexed optical nanoplasmonic  $H_2$  sensor to close this gap. Specifically, waveguide illumination of seven nanoparticle arrays made from rationally selected plasmonic hydride-forming<sup>32,56</sup> and catalytic-plasmonic<sup>57</sup> metals and alloys is combined with 64-pixel photodiode readout, producing 64 virtual material pixels through optical convolution. Coupled to a tailored transformer deep-learning model pipeline, the device accurately quantifies 0.085 – 4 vol.%  $H_2$  during a simulated Jakarta day with dynamically varying RH and CO,  $CO_2$  and  $NO_x$  contamination derived from real weather and air-quality data.<sup>58,59</sup> As a second key advance, the same model also quantifies the contaminants and delivers concentration readings of the dynamically varying contaminant species during the day, although the sensing materials were selected exclusively for  $H_2$  detection. Finally, this work advances the machine learning domain by using attention across feature blocks that

correspond to different materials on the sensor, which enables the generation of attention maps that reveal which virtual or physical sensing regions have received the largest weight at a given sensing condition, and how that weighting redistributes when the sensing environment dynamically evolves. Hence, we have introduced attention not as a generic machine learning add-on, but as a way of connecting sequence inference directly back to array design and material function, to enable further optimization and tailoring of physical active sensing materials in future sensor implementations.

## Results and Discussion

### *Realistic H<sub>2</sub> sensor operation conditions, sensor device design and active material selection*

We first defined a realistic operating envelope for H<sub>2</sub> leak-detection and safety sensing using atmospheric data from Jakarta, Indonesia, recorded during Nov. 30 – Dec. 07, 2025.<sup>58,59</sup> This setting combines high, dynamically varying RH with high levels of contamination due to heavy traffic (**Figure 1a**). Specifically, species known to compromise H<sub>2</sub> sensors through cross-sensitivity, deactivation or poisoning<sup>32</sup> i.e. CO, CO<sub>2</sub>, NO<sub>2</sub> and H<sub>2</sub>O, spanned 0.1–9.1 ppm, 438–525 ppm, 5–91 ppb and 46–97% RH, respectively. To illustrate how such environments perturb plasmonic H<sub>2</sub> sensing, we fabricated quasi-random nanodisk arrays of pure Pd<sub>100</sub>,<sup>60,61</sup> pure Pt<sub>100</sub><sup>57</sup> and a ternary Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub><sup>62,63</sup> alloy, respectively, by Hole-Mask Colloidal Lithography<sup>64</sup> and monitored their H<sub>2</sub> response through the spectral shift of the localized surface plasmon resonance (LSPR) peak centroid,  $\Delta\lambda_C$ .<sup>65</sup> Measurements in pure Ar, 80% RH synthetic air and dry synthetic air containing 200 ppm CO revealed material-dependent changes in response sign, amplitude and apparent kinetics (**Figure 1b**). Thus, the contaminants do not simply suppress sensor performance; they reshape the response in a material-specific manner. Because the apparent response times are convoluted with the gas-exchange time of the optical flow reactor, these kinetic effects are likely underestimated.

To create a nanoplasmonic H<sub>2</sub> sensor that can operate in this challenging environment, we designed a miniaturized device that treats *both* the material-specific response to H<sub>2</sub> and the material-specific cross-

sensitivity to interferant species as information rather than treating cross-sensitivity as a problem. The device comprises a black-anodized aluminum chamber with a free volume of  $\sim 1.12$  mL, gas inlet and outlet, mass-flow controllers and a humidification system (**Figure 1c**, **Figure S1**; **Methods**). An 85 mm  $\times$  12 mm  $\times$  0.5 mm fused-silica sensor chip seals the chamber and serves as a waveguide for white-light illumination, while scattered light is collected by a 64-pixel photodiode array mounted above the chip. The chip integrates six plasmonic  $H_2$ -sensing materials and one reference material: (i)  $Pd_{100}$  for its strong optical response to  $H_2$  due to hydride formation,<sup>61</sup> (ii)  $Pt_{100}$  for catalytic-plasmonic  $H_2$  sensing at high RH,<sup>57</sup> (iii)  $Pd_{70}Au_{30}$  for ultrafast<sup>66</sup> and hysteresis-free response to  $H_2$ ,<sup>67</sup> (iv)  $Pd_{87}Pt_{13}$ , (v)  $Pd_{72}Au_{14}Pt_{14}$  and (vi)  $Pd_{70}Au_{25}Cu_5$  for  $H_2$  sensing in contaminant-rich backgrounds,<sup>63</sup> and (vii)  $Au_{100}$  as a non-reactive optical reference for thermal and mechanical perturbations.<sup>55,68</sup> These materials were patterned as parallel 0.5 mm-wide nanoparticle-array strips separated by 6.25 mm, where each strip constitutes a quasi-random array of disk-shaped nanoparticles fabricated by electron-beam lithography (**Figure 1c–e**; **Methods**). Alloy formation was induced by high-temperature solid-state diffusion after sequential metal evaporation (**Figure 1f**).<sup>69</sup>

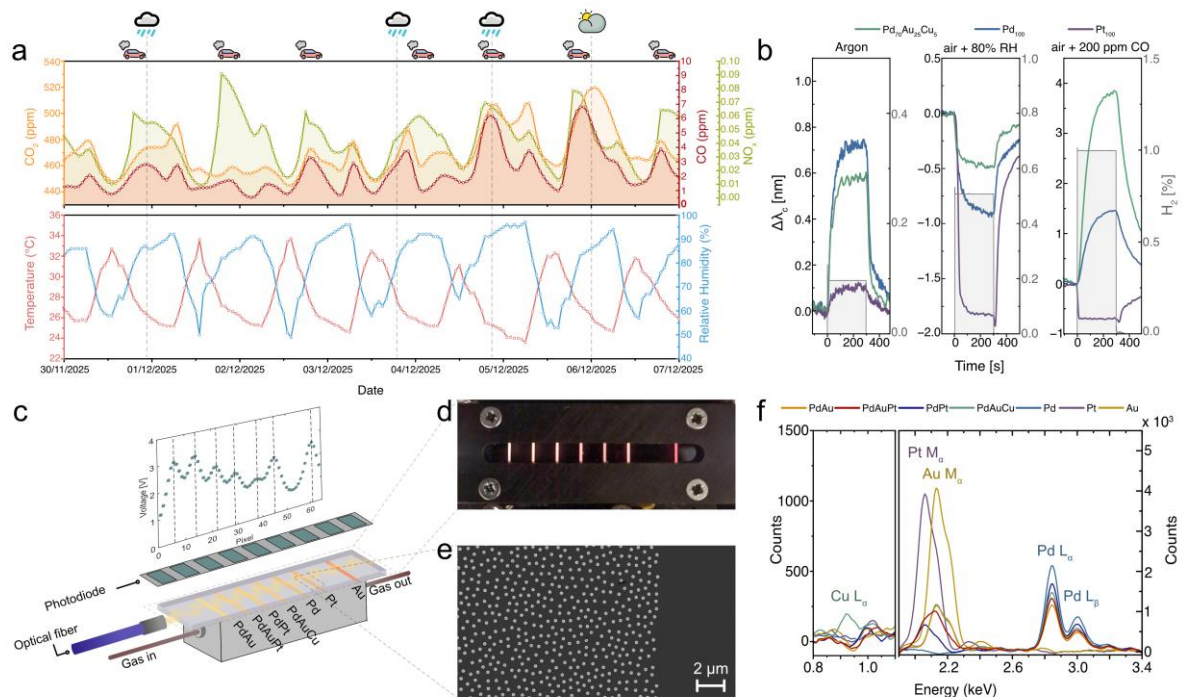


**Figure 1. Sensor operation environment in Jakarta, Indonesia, sensor design and sensing material performance.** (a) Example of real operation conditions for a  $H_2$  sensor deployed in the tropical, metropolitan area of Jakarta, Indonesia. These conditions include varying levels of  $CO_2$ ,  $CO$ ,  $NO_x$ , temperature and relative humidity

(RH), and are presented over the span of a full week, as taken from Open-Meteo, for Nov. 30 – Dec. 07, 2025 in Sunda Kelapa, Jakarta, Indonesia<sup>58,59</sup>. (b) Spectral shift of the LSPR peak<sup>65</sup>,  $\Delta\lambda_C$ , of three quasi-random arrays of Pd, Pt and ternary Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub> alloy 210 x 25 nm nanodisks fabricated by Hole-Mask Colloidal lithography<sup>64</sup> (see **Methods**) in Ar, 80% RH synthetic air and in dry synthetic air with 200 ppm CO. A 5-point moving mean has been applied to the plotted data to enhance their visual clarity. (c) Schematic depiction of the miniaturized sensor device developed for material-multiplexed plasmonic H<sub>2</sub> sensing, comprised of a small chamber with a gas inlet connected to mass-flow controllers and a gas humidifying setup. The chamber is sealed by the fused silica sensor chip, which serves as a waveguide for the illumination of the seven different sensing material nanoparticle arrays indicated, via light coupling from the optical fiber mounted towards one edge of the chip. The readout of the chip is facilitated by a 64-pixel photodiode array mounted on top, which collects the light scattered from the seven physical nanoparticle arrays and the optically convoluted virtual materials in between (see **Methods** for details). (d) Top-view photograph of the sensor device without the photodiode mounted, revealing the light scattered from the nanoparticle array “strips” upon illumination via the waveguide. We note that the slightly different tints of the different arrays reflect their different material compositions, i.e., from left to right: Pd<sub>70</sub>Au<sub>30</sub>, Pd<sub>72</sub>Au<sub>14</sub>Pt<sub>14</sub>, Pd<sub>87</sub>Pt<sub>13</sub>, Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub>, Pd<sub>100</sub>, Pt<sub>100</sub>, Au<sub>100</sub> (e) Top-view SEM micrograph of the edge of a Pt<sub>100</sub> nanoparticle array. Note the quasi-random distribution of the nanoparticles implemented by electron beam lithography. The scale bar is 2  $\mu$ m. For representative high-magnification SEM micrographs for every nanoparticle system, see **SI Figure S2**. (f) Background-subtracted SEM-EDX spectra of the 7 nanoparticle arrays. A 5-point moving mean has been applied to the plotted spectra to enhance their visual clarity. For the non-background corrected spectra of the full energy range and nominal vs measured compositions, see **SI Figure S3**, **S4**, respectively.

### *Virtual-material-multiplexed sensor readout*

We next tested whether the optical readout itself provides virtual material multiplexing via optical convolution. Comparing the seven-material chip with a control chip containing three Au nanoparticle-array strips only showed that scattered light intensity is indeed strongest above each physical material strip but remains detectable several pixels away (**Figure 2a**). Thus, each photodiode pixel records a distinct optical convolution of signals from several nanoparticle arrays, generating 64 virtual material pixels from only seven physical sensing regions. This architecture thus generates a rich, spatially structured response for deep-learning analysis while retaining simple hardware implementation. For discussion, we nonetheless assign material labels (Pd<sub>100</sub>, Pd<sub>70</sub>Au<sub>30</sub>, etc.) to the central pixel  $\pm 1$  above each physical strip, although these pixels also contain residual optical mixing (**Figure 2a**).

With this nomenclature established, we exposed the sensor to mixed pulses of H<sub>2</sub>, CO, CO<sub>2</sub> and NO in dry synthetic air, followed by a humid section containing all contaminants at 40% RH (**Figure 2b,c**). NO was chosen instead of NO<sub>2</sub> because it binds most strongly to Pd and therefore provides the strongest deactivation challenge for Pd-based materials.<sup>70,71</sup> We find that H<sub>2</sub> exposure generally produced the expected concentration-dependent decrease in photodiode voltage, consistent with reduced light scattering upon H absorption in Pd-based systems. In contrast, Pt was largely insensitive to H<sub>2</sub> under dry conditions and followed the slow baseline drift of the inert Au reference (**Figure 2b,c**).<sup>72-74</sup>

As a second aspect, it is clear that the contaminants strongly reshaped the sensor response. Under varying CO (region I), the smallest H<sub>2</sub> pulses, 0.085 and 0.15 vol.%, were no longer clearly resolved (**Figure 2d**). With combined CO and CO<sub>2</sub> (region II), only selected materials responded to 0.5 and 1.0 vol.% H<sub>2</sub>, whereas others remained deactivated and showed slow baseline drift (**Figure 2e**). Increasing RH from 0% to 40% (region III), induced pronounced material-dependent baseline shifts and cross-sensitivity to all contaminants (**Figure 2f,g**). Together, these data show that optical convolution and contaminant cross-sensitivity generate a high-dimensional virtual-material response that can be exploited using a suitable deep-learning model.

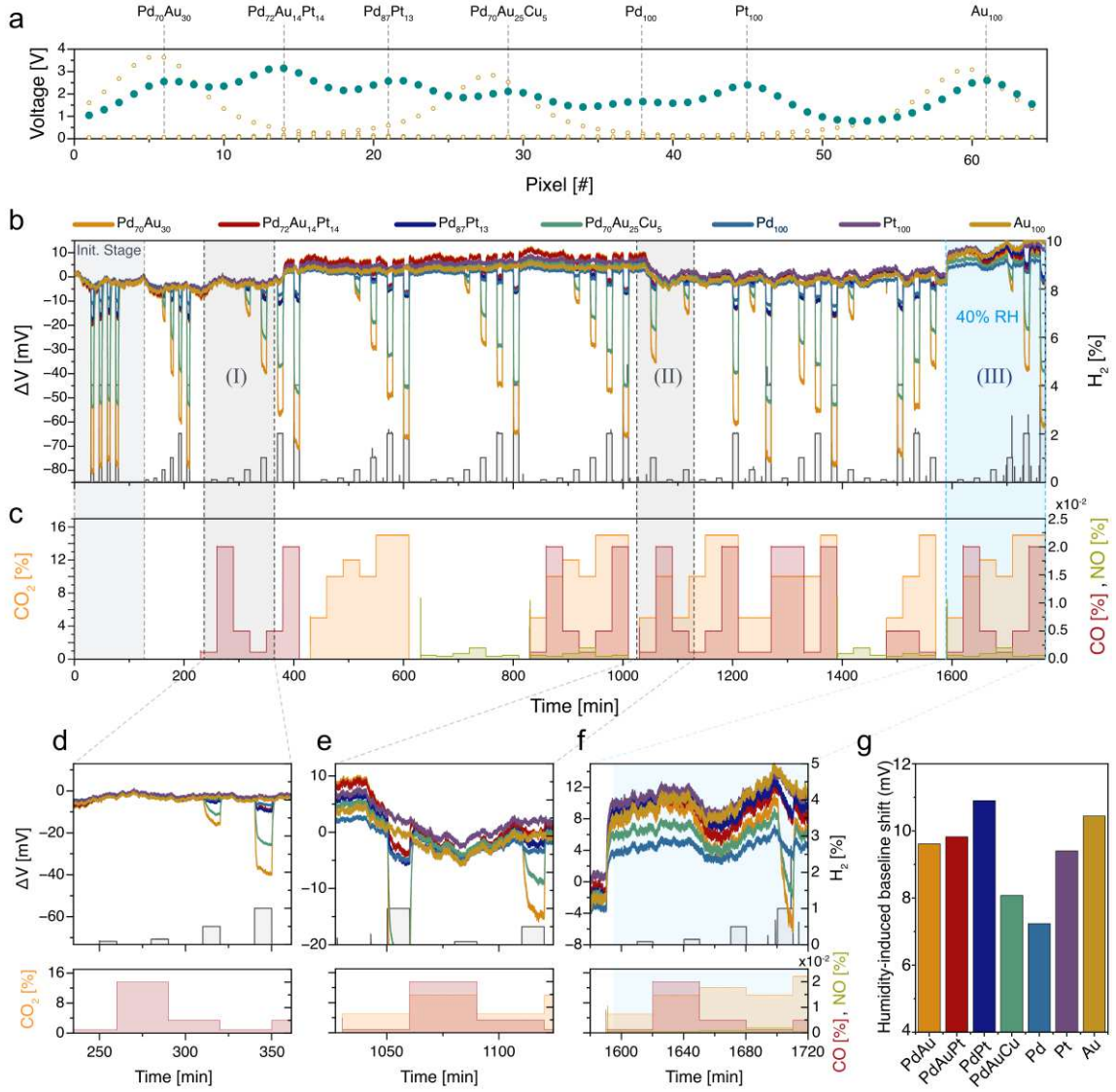


**Figure 2. Photodiode array readout to pulsed mixtures of H<sub>2</sub>, CO, CO<sub>2</sub> and NO in synthetic air.** (a) Photodiode voltage signal proportional to scattered light intensity recorded by each of the 64 pixels for a sensor chip with Pd<sub>70</sub>Au<sub>30</sub>, Pd<sub>72</sub>Au<sub>14</sub>Pt<sub>14</sub>, Pd<sub>87</sub>Pt<sub>13</sub>, Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub>, Pd<sub>100</sub>, Pt<sub>100</sub>, Au<sub>100</sub> nanoparticle array strips (teal) and a chip with three Au<sub>100</sub> strips (yellow). Dashed lines depict pixels located atop each physical material. (b) Response of the pixels atop  $\pm 1$  the Pd<sub>70</sub>Au<sub>30</sub>, Pd<sub>72</sub>Au<sub>14</sub>Pt<sub>14</sub>, Pd<sub>87</sub>Pt<sub>13</sub>, Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub>, Pd<sub>100</sub>, Pt<sub>100</sub>, Au<sub>100</sub> nanoparticle array strips to H<sub>2</sub> pulses in the range of 0.085 – 4 vol.% in dry synthetic air and in 40 % RH synthetic air during the last 3 h (blue rectangle) and in different levels of contamination by CO<sub>2</sub>, CO, and NO in the ranges of 2 – 15 vol.%, 0.001 – 0.02 vol.% (10 – 200 ppm), and 0.0002 – 0.002 vol.% (2 – 20 ppm), respectively, as depicted in panel (c). (d) Zoom-in on the gray-shaded CO-contaminated section (I) in panels (b) and (c), revealing that the smallest H<sub>2</sub> pulses are not clearly resolved. (e) Zoom-in on the gray-shaded CO- and CO<sub>2</sub>-contaminated section (II) in panels b and c, revealing for slightly higher H<sub>2</sub> concentration pulses how only selected materials exhibit distinct response, while all others remain deactivated towards H<sub>2</sub> but exhibit slow baseline drift. (f) Zoom-in on the blue-shaded CO-, CO<sub>2</sub>- and NO contaminated section (III) region where RH is increased from 0% to 40%, revealing an RH-induced baseline shift of all materials and distinct cross-sensitivities to the other contaminants. (g) Bar plot revealing the baseline shift due to an RH increase from 0% to 40% by the different materials on the sensor chip.

To decode the high-dimensional response of the 64 virtual material pixels, we developed an encoder-only transformer that operates directly on the full 64-pixel optical time trace (**Figure 3**). After baseline correction, normalization and temporal windowing, each time window is represented as an input sequence  $S$  of size  $T \times 64$ , in which  $T$  is the sequence length and the 64 columns each correspond to an individual pixel of the photodiode array (**Figure 3a; Methods**). This preserves both the temporal evolution of the signal and the fixed hardware mapping between optical readout position and virtual sensor material. This retained optical convolution is the central machine-learning representation used in the model: the 64-pixel readout is treated as a structured virtual-material basis, rather than reduced to material-averaged traces before training.

Each 64-dimensional optical feature vector is then projected into a shared latent space, combined with positional encoding, and processed by stacked transformer encoder blocks that learn temporal dependencies and cross-pixel interactions across the full sequence (**Figure 3b**). This architecture is especially well suited to the present problem because the relevant information is distributed both across time and across partially overlapping virtual material features, rather than being localized to a single material or a single steady-state descriptor. The resulting encoder representation is then read out by gas-specific regression heads that predict the concentration time traces of H<sub>2</sub>, CO, CO<sub>2</sub> and NO as functions of time. These gas-specific output heads are distinct from the model's internal self-attention heads; in principle, additional analytes could be accommodated by extending the output layer and retraining on the corresponding target time traces. The model is therefore trained end-to-end on preprocessed optical sequences and analyte concentration targets, with the loss applied only to the analyte time traces, leading to emergent interpretable properties (**Figure 3c**).

The central methodological novelty here is that the transformer exploits two coupled levels of multiplexing: physical material multiplexing on the chip and optical virtual-material multiplexing in the readout. Because the model learns directly from this physically grounded, optically mixed sensing manifold, cross-sensitivity and optical convolution are treated as information rather than as artifacts to

remove. Secondly, to enable interpretation of which (virtual) material pixels that are given most weight by the trained model in different sensing conditions, it enables the extraction of head-averaged “attention maps” and grouping them according to the pixels of the photodiode array (**Figure 3b,c**). Hence, these attention maps provide a model-based view of which pixels and time intervals that contribute most strongly to the encoder’s predictions at a given condition. In that sense, the attention analysis links temporal sequence decoding back to the (virtual) nanoparticle arrays on the sensor and provides a route to evaluating how the virtual material feature space is used under different conditions.

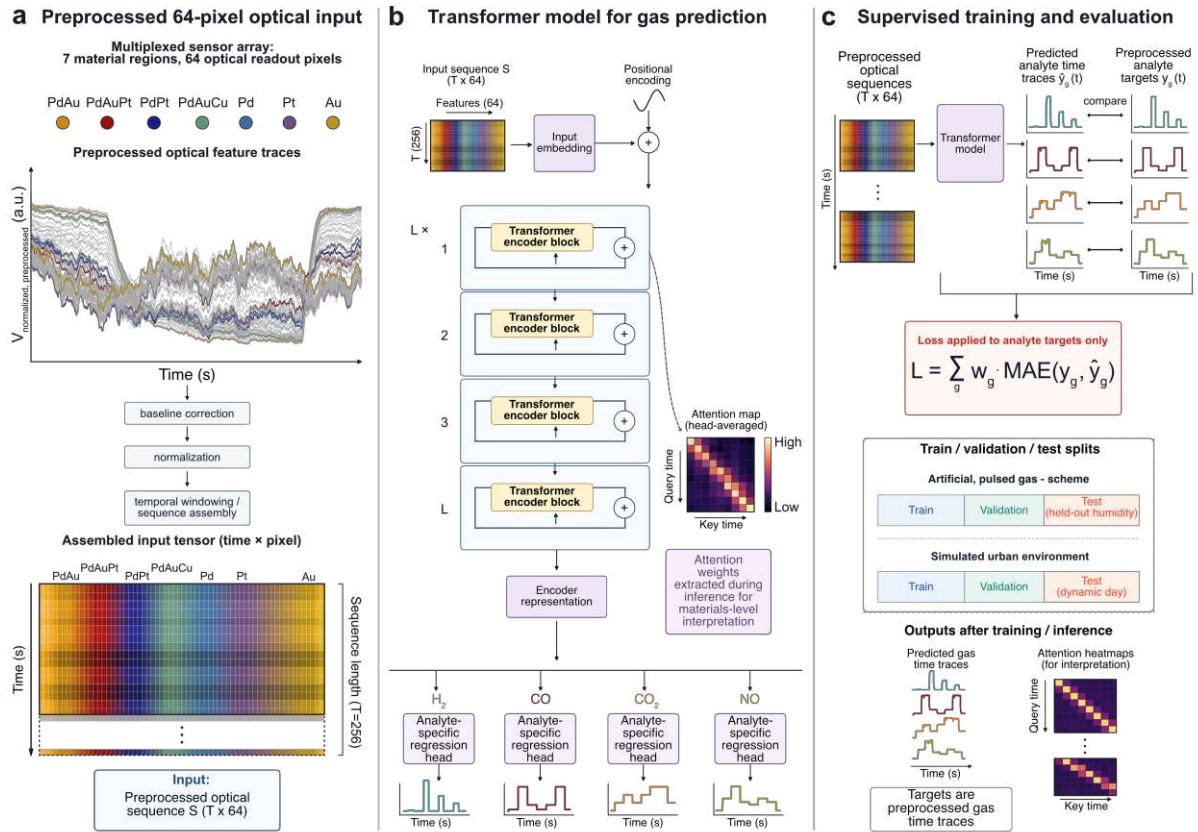


**Figure 3. Transformer workflow for analyte decoding from a multiplexed optical nanoplasmonic sensor.**

(a) Preprocessed 64-pixel optical input. The seven physical and optically convoluted virtual nanoparticle-array material regions are read out by 64 photodiode pixels, generating preprocessed optical feature traces that are baseline-corrected, normalized and assembled into an input sequence (T x 64). The 64 features correspond to fixed optical readout pixels and retain the optically convoluted virtual-material response. (b) Encoder-only transformer model for multiple analyte concentration prediction. Each 64-dimensional optical vector is embedded, combined with positional encoding and processed by stacked transformer encoder blocks. The shared encoder representation is read out by gas-specific regression heads to predict  $H_2$ ,  $CO$ ,  $CO_2$  and  $NO$  analyte concentration

trajectories, while head-averaged attention maps are extracted during inference for pixel- and material-level interpretation. (c) Supervised training and evaluation. The model is trained on preprocessed optical sequences and time-aligned analyte concentration targets, with the loss applied to the analyte targets only. Train/validation/test splits are defined for the dry multi-analyte held-out humidity test and the humid dynamic multi-analyte test; after training, predicted analyte trajectories and attention heatmaps are evaluated on held-out measurements.

### *Predicting gas concentrations with the transformer in an artificial pulsed-gas scheme*

We first evaluated the transformer in an artificial, deliberately demanding pulsed-gas scheme containing 0 – 4% H<sub>2</sub>, 0 – 0.02% CO, 0 – 15% CO<sub>2</sub> and 0 – 0.002% NO in synthetic air. The contaminant concentrations were intentionally higher than typical urban-air levels (cf. **Figure 1a**) to stress-test the sensor under severe interference. The model was trained on three identical 0% RH step-pulse measurements (**SI Section S5–S7**) and evaluated on a held-out separate test sequence (**Figure 4**). Before H<sub>2</sub>O introduction, where the test conditions matched the training regime, the model accurately predicted H<sub>2</sub> concentrations (**Figure 4a**). Specifically, defining the relative error of the predictions as  $\left| \frac{x_p - x_t}{x_p} \right|$ , where  $x_t$  is the target concentration and  $x_p$  is the mean predicted gas concentration over the last 12 prediction data points for every pulse, the model yielded a mean relative error of 0.8% at the end of each pulse over all H<sub>2</sub> pulses completed before H<sub>2</sub>O introduction (**Figure 4b**). It also quantified CO, CO<sub>2</sub> and NO with mean relative errors of 2.3%, 1.8% and 1.7%, respectively (**Figure 4c–e**), and outperformed static ridge and GRU baselines for every gas channel (**Supplementary Tables S4 and S6**). To also test the out-of-distribution performance of the DL model, we introduced 40% RH in the final 3 hours of the test sequence (**Figure 4a**), which reduced prediction accuracy, as expected for an out-of-distribution condition,<sup>75</sup> but the model still detected most gas pulses correctly (“H<sub>2</sub>O introduction region” in **Figure 4a–e**).

We next used the transformer attention maps to identify which parts of the virtual-material readout were most important for the prediction. Attention was aggregated over the 64 pixels (**Figure 4f**) and, for discussion, we again assigned the physical materials to the pixels located atop  $\pm 1$  each physical material strip (**Figure 4g**), acknowledging that these pixels still contain residual optical convolution. In the 0%

RH region, the model placed the largest mean attention weight on Pd<sub>70</sub>Au<sub>30</sub> (17.7%), consistent with its reported strong response to H<sub>2</sub> in dry air<sup>66,67,75,76</sup> (**Figure 2b**) and lower NO and CO adsorption energies compared with Pd<sub>100</sub>, rendering it less prone to complete deactivation.<sup>77</sup> Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub> received the second-highest attention (9.8%), in line with its strong response in dry air (cf. **Figure 2b**) and reported resistance to CO and CO<sub>2</sub> poisoning.<sup>63</sup>

Notably, the remaining 58.3% of the total attention was assigned to fully virtual material regions *between* the physical strips (**Figure 4g**), where optical convolution is strongest. Specifically, even when corrected for the number of pixels in each category, pixels assigned to the fully virtual materials still carried a mean of 1.4% relative attention per pixel (43 pixels) compared to the 2.0% relative attention per pixel (21 pixels) assigned to the physical materials (**SI Section S11; Table S3**). This conclusion is further supported by physical-pixel masking experiments in an ablation study (**SI Section S12**) and by transient attention spikes above 15% between Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub> and Pd<sub>100</sub> in regions *without* H<sub>2</sub>, but with high concentrations of NO (**Figure 4f**). Hence, the virtual-material multiplexing based on optical signal convolution demonstrated here provides information that would be lost in conventional e-nose designs based on isolated sensors or serially connected devices.<sup>8,14-16,24,25</sup>

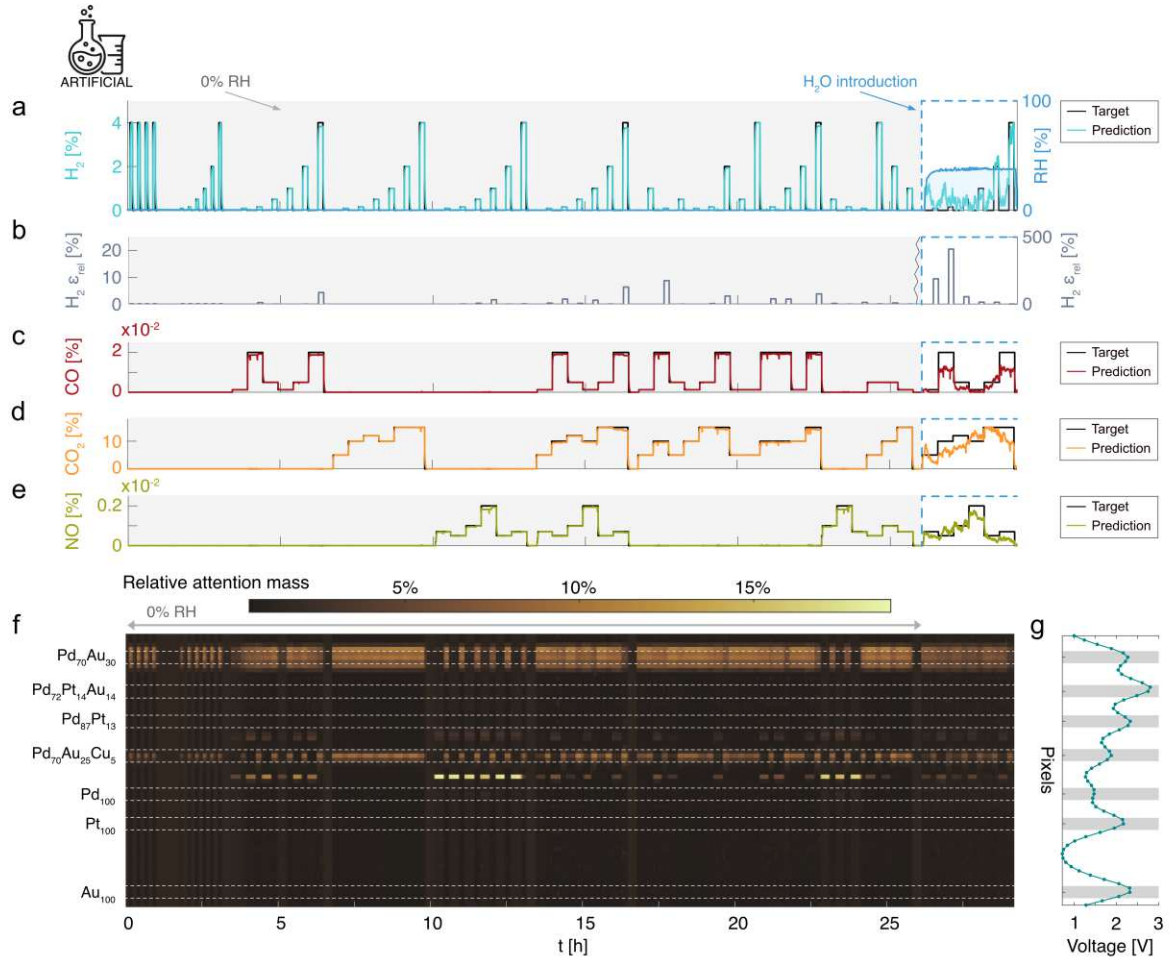


**Figure 4. Concentration predictions in pulsed mixtures of CO, CO<sub>2</sub>, NO and H<sub>2</sub> in synthetic air and pixel attention map.** (a) Target and predicted concentrations for H<sub>2</sub>. Humidity in % RH is indicated by light blue shading. (b) The relative error of the H<sub>2</sub> predictions, defined as  $\epsilon_{rel} = \left| \frac{x_p - x_t}{x_p} \right|$ , where  $x_t$  is the target concentration and  $x_p$  is the mean predicted H<sub>2</sub> concentration from the last 12 prediction data points for every pulse. Note the different scales in the 0% RH region (left axis) and the humid region (right axis). Target and predicted concentrations for (c) CO, (d) CO<sub>2</sub> and (e) NO. In panels (b-e), the 0% RH region is indicated with a grey shaded background and the region where RH is above 0% is indicated by the dashed, light-blue box. (f-g) DL model feature attention map (f) and light scattering profile from the sensor chip (g). The attention profiles from pixels atop  $\pm 1$  the seven physical material arrays on the sensor chip are outlined by the white dashed lines. Note the transiently high attention of the DL model to fully virtual materials localized between the physical ones.

### *Predicting gas concentrations in a simulated, high-humidity, poor air-quality urban area*

We next tested the same transformer architecture under realistic urban-air conditions simulated in the lab. The model was trained on two protocol segments, each comprising a 3 h initialization followed by a 27 h Jakarta day-simulation sequence based on real atmospheric data from Nov. 15 and 23, 2025 (**SI Section S8–S10**).<sup>58,59</sup> It was then evaluated on a held-out 24 h long Jan. 5, 2026 sequence with CO, CO<sub>2</sub> and NO varying between 0.4–7.0 ppm, 444–527 ppm and 9–70 ppb, respectively (**Figure 5a–c**), including two simulated rush-hour periods, and RH slowly varying between 61% and 98% (**Figure 5d**). This test is more demanding than the pulsed scheme above because high RH strongly poisons Pd-based H<sub>2</sub> sensors<sup>32,75,78</sup> and because humidity and contaminants co-vary *continuously* rather than appearing as isolated pulses.

Despite these challenging conditions, the model quantified CO, CO<sub>2</sub> and NO with mean relative errors of 5.0%, 6.6% and 8.4%, respectively (**Figure 5a–c**). It also quantified H<sub>2</sub> throughout the full sequence with a mean relative error of 3.8% at the end of the pulses (**Figure 5d,e**). Errors were largest during humid morning and evening periods, when all interferents were highest, reaching a mean pulse-end relative error of 5.0% (**Figure 5e**). By contrast, during the lower-contamination midday period, when RH also decreased, the H<sub>2</sub> error fell to 0.3% for all pulses and to 0.1% for pulses above 0.1% H<sub>2</sub> (**Figure 5e**). Notably, this accuracy was achieved although RH never dropped below 60%. The largest relative error, 25.5%, occurred for the lowest H<sub>2</sub> pulse, 0.085%, at  $t = 00:30$  min under high morning humidity and contamination (**Figure 5a–d**). Even then, the model predicted 0.107% H<sub>2</sub>, corresponding to an absolute error of 0.022% H<sub>2</sub>. Restricting the analysis to pulses above the 0.1% H<sub>2</sub> limit-of-detection target set by the US Department of Energy<sup>79</sup> reduced the maximum relative error to 7.5%, with a maximum absolute error of 0.275% H<sub>2</sub>. Extended physical-unit ranges and pulse-plateau error summaries for both held-out regimes are provided in Supplementary Note 3 (**Tables S8–S12**). The transformer also outperformed both static ridge and GRU baselines for all four output channels in this held-out Jakarta sequence (**Supplementary Tables S5 and S7**).

Next, attention analysis revealed a broader material dependence than in the pulsed-gas experiment in dry conditions (**Figure 5f**, cf. **Figure 4f**). Specifically, instead of concentrating on Pd<sub>70</sub>Au<sub>30</sub>, attention is now spread across Pd<sub>87</sub>Pt<sub>13</sub>, Pd<sub>72</sub>Au<sub>14</sub>Pt<sub>14</sub>, Pd<sub>70</sub>Au<sub>30</sub> and Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub>. Using again the pixels atop  $\pm 1$  each physical strip as material proxies (**Figure 5g**), Pd<sub>72</sub>Au<sub>14</sub>Pt<sub>14</sub> received the highest mean attention over the full sequence (12.2%), followed by Pd<sub>87</sub>Pt<sub>13</sub> (10.6%) and Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub> (10.4%). This corroborates our selection of these alloys for H<sub>2</sub> sensing under high CO, NO and H<sub>2</sub>O backgrounds and highlights the value of Pt-containing alloys at high RH.<sup>57</sup> As RH and contaminant levels decreased around noon, attention to Pd<sub>70</sub>Au<sub>30</sub> increased from 3.7% to 6.9% (**Figure 5f**), consistent with its favorable dry-condition response (**Figure 4f**), whereas Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub> became more prominent during the high-contaminant morning and evening periods. Taken together, the revealed attention clearly demonstrates the benefit of the different alloys under varying atmospheric regimes. Following this line, the dominance of *alloy* regions over pure Pd<sub>100</sub>, Pt<sub>100</sub> and Au<sub>100</sub> is consistent with the established benefits of alloying for H<sub>2</sub> sensing, where the constituent metals act synergistically.<sup>35,36,47,62,63,67,72,80-88</sup> In the present sensor, this chemical alloying is further leveraged by virtual-material multiplexing whose importance is highlighted by the model's attention being broadly *distributed* around Pd<sub>87</sub>Pt<sub>13</sub> and extending toward neighboring Pd<sub>72</sub>Au<sub>14</sub>Pt<sub>14</sub> and Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub> regions, and further supported by the ablation study (**SI Section S12**). This virtual-alloying concept is therefore central to the simultaneous quantification of H<sub>2</sub>, CO, CO<sub>2</sub> and NO demonstrated here.

As a final note, and like previous transformer-based acceleration of plasmonic H<sub>2</sub> readout<sup>87</sup>, response times extracted from the model-predicted H<sub>2</sub> trace collapse to approximately one prediction time step, which corresponds to  $\sim 5$  s. Furthermore, these response times become nearly H<sub>2</sub> concentration independent, whereas  $t_{50}$  values extracted directly from individual optical material-strip signals remain material- and concentration-dependent (**SI Section S13**).

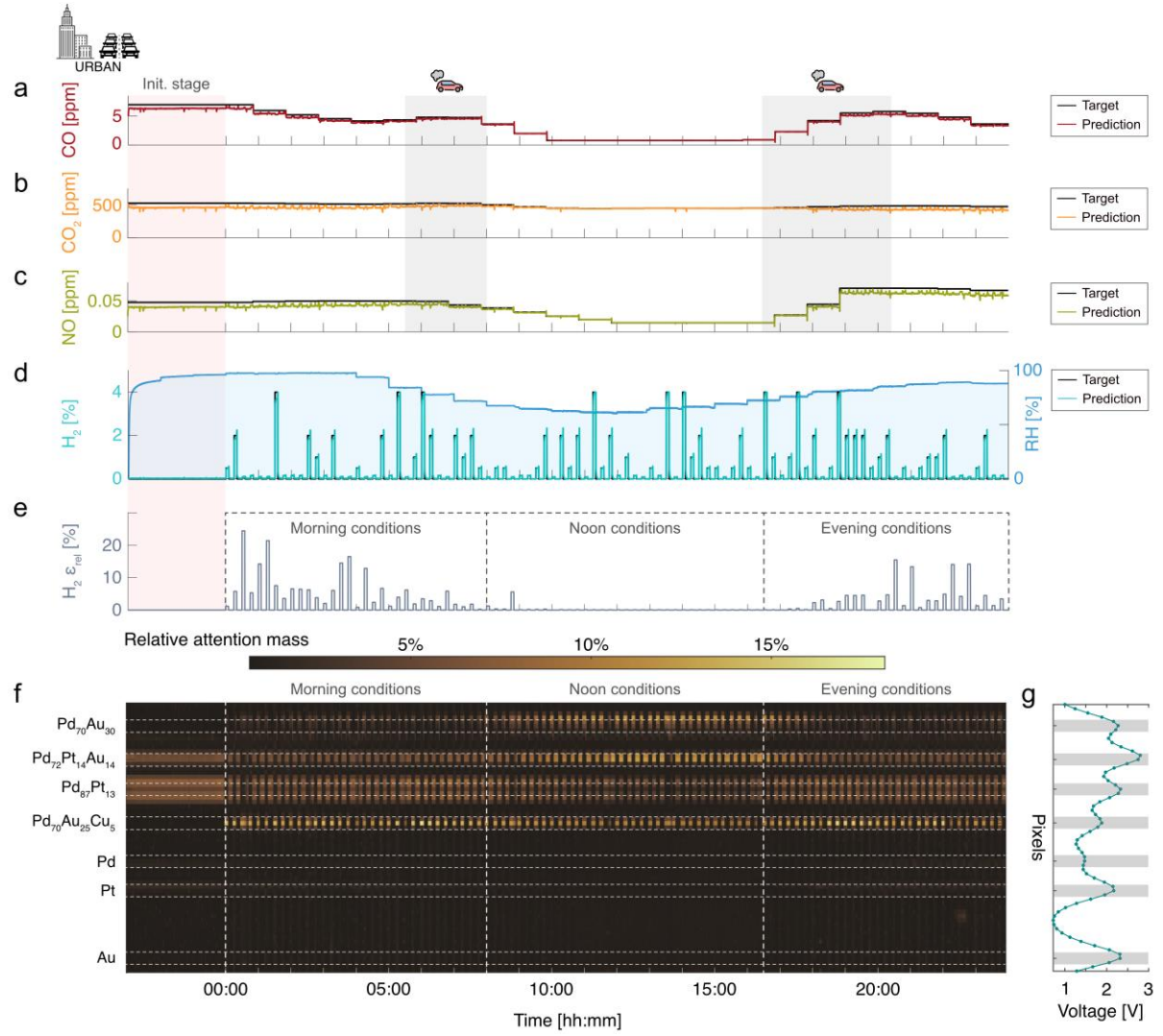


**Figure 5. CO, CO<sub>2</sub>, NO and H<sub>2</sub> concentration predictions and pixel attention map for a held-out Jakarta urban-air simulation.** Target and predicted concentrations for (a) CO, (b) CO<sub>2</sub>, (c) NO and (d) H<sub>2</sub> during the 27 h Jakarta day-simulation sequence based on the real weather and contamination conditions of the Indonesian capital Jakarta on Jan. 5 2026.<sup>58,59</sup> The %RH is indicated by a light blue shadow in (d). A 3 h initialization to stabilize the gas flows is indicated with red-shaded background in (a-e). Two simulated, traffic “rush-hour” segments are indicated with a grey-shaded background in (a-c). (e) The relative error of the H<sub>2</sub> predictions, defined as  $\varepsilon_{rel} = \left| \frac{x_p - x_t}{x_p} \right|$ , where  $x_t$  is the target concentration and  $x_p$  is the mean predicted H<sub>2</sub> concentration from the last 12 prediction data points for every pulse. (f-g) DL model feature attention map (f) and light scattering profile from the sensor chip (g). The attention profiles from pixels atop  $\pm 1$  the seven physical material arrays on the sensor chip are outlined by the white dashed lines in (f) and grey-shaded areas in (g). Morning (00:00-08:00), noon (08:00-16:30) and evening (16:30-23:59) conditions are defined in (e-f). We highlight the transiently high attention of the DL model to fully virtual materials localized between the physical ones and the generally high attention on alloys rather than pure metals, corroborating the well-established advantage of alloying in H<sub>2</sub>-sensing applications, where the properties of individual metals act synergistically in complex chemical environments.

## Conclusions

We have introduced a quantitative, transformer-augmented and virtual-material-multiplexed plasmonic H<sub>2</sub> sensor for chemically deactivating humid air environments, which constitutes one of the practically most important deployment scenarios for H<sub>2</sub> safety sensors. On the hardware side, our device combines a multiplexed waveguide-based sensor device comprising seven rationally selected plasmonic metal nanoparticle arrays made from Pd<sub>70</sub>Au<sub>30</sub>, Pd<sub>72</sub>Au<sub>14</sub>Pt<sub>14</sub>, Pd<sub>87</sub>Pt<sub>13</sub>, Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub>, Pd<sub>100</sub>, Pt<sub>100</sub> and Au<sub>100</sub>, respectively. They are multiplied into 64 unique virtual sensing materials by optical convolution and read-out by a 64-pixel photodiode array. On the data analysis side, we have developed an encoder-only transformer deep-learning algorithm that operates on the highly complex and information-rich 64-pixel optical time trace generated by the sensor. This combined solution challenges existing gas sensing concepts as it not only can *classify* H<sub>2</sub> in a chemically highly deactivating environment but accurately *quantifies* H<sub>2</sub> in simulated Jakarta urban air with up to 98% RH and simultaneous CO, CO<sub>2</sub> and NO contamination. For H<sub>2</sub> pulses above the 0.1% limit-of-detection target set by the US DoE,<sup>79</sup> the maximum relative error was 7.5%, satisfying the ISO 26142:2010 standard<sup>89</sup> demanding  $\pm 25\%$  accuracy criterion for stationary H<sub>2</sub> detection even during the most strongly deactivating morning and evening rush-hours conditions with peaking RH. As a second key advance, by leveraging cross-sensitivity, the same model also quantified CO, CO<sub>2</sub> and NO with average relative errors of 5.0%, 6.6% and 8.4%, respectively, despite the sensing materials being selected for H<sub>2</sub> sensing rather than contaminant detection.

Beyond analyte quantification, the attention maps provided by the transformer deep learning model link model inference to sensor design and material selection. They show that attention broadens across virtual materials as the chemical environment becomes more complex, and that alloy regions, especially ternary alloys, dominate over pure metals, consistent with the synergistic role of alloying in H<sub>2</sub> sensing, and that strongly convolved pixels between physical material strips carry substantial information. This confirms the practical value of virtual sensing materials generated by optical convolution and has two important future consequences: (i) it facilitates the design of highly virtually material-multiplexed sensor devices for the simultaneous detection of a large number of analytes without the costly and

technically challenging demand for physical implementation of a large number of real sensing materials; (ii) it opens for future sensing material optimization based on input collected from sensors deployed in the field. The latter will directly link research and development with field-deployed sensor systems and has thereby the potential to further revolutionize the way we design and improve sensors in the future.

## Methods

*Sensor device:* The sensor device used for all measurements consists of an aluminum-body chamber dyed black to reduce light scattering from the inside with a volume of ~1.12 mL and in- and outlets for gas flow. It is equipped with a set of Mass Flow Controllers (MFCs, Bronkhorst High-Tech B.V.) that control the flow rate and gas composition (synthetic air, H<sub>2</sub>, CO, CO<sub>2</sub> and NO), a Liquid Flow Controller (LFC, Bronkhorst High-Tech B.V.) for controlling the water supply rate, and a Controlled Evaporator Mixer (CEM, Bronkhorst High-Tech B.V.) that humidifies the gas. In the first sensor performance measurements (**c.f. Figure 2, Figure 4**) the water supplied from the LFC into the CEM for humidifying the gas stream (40% RH) in the last 3 hours of the measurement is referenced at T=30 °C, 1,013 bar, and 200 mL/min total gas flow rate. In the 27 h Jakarta urban air simulation measurement (**c.f. Figure 5**), the water supplied from the LFC into the CEM for humidifying the gas stream is referenced to RH values at the corresponding reported hourly real temperature data<sup>59</sup>, 1.013 bar pressure and 350 mL/min total gas flow rate. In both cases the calculation was performed using Bronkhorst's Fluidat software. The true humidity level was measured by a calibrated humidity and temperature probe (HMP7,TMP1, Vaisala Oyj) positioned at the chamber outlet. The reactor temperature was controlled using a Peltier element (RS PRO Peltier-module, RS Components GmbH) and a closed-loop temperature control system (Eurotherm 3216) in a feedback loop manner, where the sample temperature inside the chamber measured by a K-type thermocouple was continuously used as the input. The fused-silica substrate with the nanoparticle arrays (the "sensor chip") acts both as the waveguide and the lid for the chamber. The nanoparticle arrays are positioned facing downwards into the chamber where they are exposed to the gas mixture. White light (AvaLight-HAL-S-Mini, Avantes BV) is coupled into the chip through an optical fiber (QP600-2-UV-VIS, Avantes BV), the evanescent field excites localized surface plasmon

resonances in the nanoparticle arrays, and the upward-scattered light is collected by a photodiode (PD) array with 64 pixels (Hamamatsu S11865-64) placed closely above the reactor (**c.f. Figure 1b,c, SI Section S1.**). The measurements in **Figures 2 & 4** were performed in synthetic air with a total flow of 200 mL/min. The Jakarta simulated urban air measurements (**c.f. Figure 5**) was performed in synthetic air with a total flow of 350 mL/min. In cases where the contaminant concentration from the real reported weather/contaminant concentration data was too low to achieve in our experimental setup, we opted for the lowest attainable concentration that the MFCs could supply, i.e., higher (and therefore more challenging) than the real concentration (**SI Section S8**). In all cases the H<sub>2</sub> concentrations used were 0.085, 0.15, 0.5, 1, 2, 4 vol.%.

*Experimental setup data displayed in Figure 1b:* The setup used for the data displayed in **Figure 1b** consists of a quartz tube plug-flow reactor with optical access for transmittance measurements (Insplorion AB). It is equipped with a set of Mass Flow Controllers (MFCs, Bronkhorst High-Tech B.V.) that control the flow rate and gas composition (Argon, synthetic air, H<sub>2</sub>, CO), a Liquid Flow Controller (LFC, Bronkhorst High-Tech B.V.) for controlling the water supply rate, and a Controlled Evaporator Mixer (CEM, Bronkhorst High-Tech B.V.) that humidifies the gas. In these measurements, the water supplied from the LFC into the CEM for humidifying the gas stream is referenced to RH values at 30 °C, 1.013 bar, and 200 mL/min total gas flow rate. Specifically, the corresponding water flow for 80% RH was 0.333 g/h and was calculated using Bronkhorst's Fluidat software. The humidity level was measured by a calibrated humidity and temperature probe (HMP7, Vaisala) positioned at the chamber inlet. The reactor temperature was controlled using a closed-loop temperature control system (Eurotherm3216) in a feedback loop manner, where the sample surface temperature inside the chamber (measured by a K-type thermocouple) was continuously used as input. The chamber can accommodate up to two samples, which are illuminated using an unpolarized halogen white light source (AvaLight-HAL-S-Mini, Avantes BV) coupled through a bifurcated optical fiber (FCB-UV600-2, Avantes BV) equipped with collimating lenses. The transmitted light from each sample is collected and analyzed by a dual-channel fiber-coupled fixed-grating spectrometer (AvaSpec-ULS2048CL-2-EVO, Avantes BV).

*Sample Nanofabrication:* Elongated sensor chips (12 mm × 85 mm) were fabricated from 6-inch fused silica wafers of 500 μm thickness. To enable reliable resist coating on the high-aspect-ratio substrates while avoiding post-fabrication contamination of the nanostructures, a backside pre-dicing strategy was employed prior to electron beam lithography (EBL). Partial dicing to a depth of 250 μm was performed from the backside of the wafer using a Disco DAD3350 equipped with a K010-600JXS blade and using a feed rate of 3 mm s<sup>-1</sup>. This approach pre-defined the final sample geometry without fully separating the chips, maintaining mechanical stability during subsequent lithographic processing. Following pre-dicing, the wafer was cleaned using standard RCA procedures. Specifically, SC-1 and SC-2 cleaning steps were carried out at 80 °C for 10 min each, followed by thorough rinsing in deionized water and nitrogen blow-drying. For EBL processing, a bilayer resist stack was applied. First, MMA(8.5)MMA-EL4 was spin-coated at 2000 rpm for 60 s (acceleration 1000 rpm s<sup>-1</sup>), followed by baking at 180 °C for 5 min on a hotplate. Subsequently, PMMA 950k A2 was spin-coated at 4000 rpm for 60 s (acceleration 2000 rpm s<sup>-1</sup>) and baked at 180 °C for 5 min on a hotplate. Due to the insulating and optically transparent nature of the fused silica substrate, a 20 nm chromium layer was deposited by thermal evaporation (Lesker Nano system) to provide charge dissipation during exposure and enable height detection within the EBL system. Patterning of disks with 210 nm in diameter, and 500 nm center-to-center distance was performed using a Raith EBPG 5200 at an acceleration voltage of 100 kV and a beam current of 30 nA, with a beam step size of 10 nm and an exposure dose of 500 μC cm<sup>-2</sup>. After exposure, the chromium layer was removed by wet etching (1 min in standard Cr etchant), followed by rinsing in deionized water and nitrogen drying. The resist was then developed in a solution of isopropanol (IPA) and water (4:1) for 60 s and immediately blow-dried with nitrogen. Subsequently, electron beam evaporation was performed on the wafer, where only one nanoparticle array was exposed at a time, while the other six were physically masked out using flat silicon pieces, that block evaporated material from reaching the wafer surface. In the cases of multi-element arrays, the evaporation was performed layer-by-layer. In all cases the total deposited thickness was 25 nm. Post metallization the wafer was submerged for 24 hours in a 1165 remover solution (“MicroPosit®”) to induce lift-off of the mask and subsequently rinsed and blow-dried with nitrogen. The individual sensor elongated sample was extracted from the pre-diced wafer by applied force at the diced positions. Finally, the sample was

annealed at 500 °C for 48 hours under a flow of 2 vol.% H<sub>2</sub> in Ar to induce alloy formation by solid-state diffusion.

*Hole-mask Colloidal Lithography:* For the sensor materials used in **Figure 1b**, masks with quasi-random array of holes with 210nm nominal diameter were fabricated using Hole-mask Colloidal Lithography<sup>64</sup>, onto  $0.9 \times 0.9 \times 0.05 \text{ cm}^3$  fused silica substrates (Siegert Wafer GmbH). Following the mask fabrication, PdAuCu (nominal 70:25:5 at.%), Pd, and Pt were deposited via electron beam evaporation (25 nm of total deposited thickness for each sensor). In the former case, the three different elements were deposited layer-by-layer. This resulted in three quasi-random arrays of 210 x 25 nm nanodisks each comprised of the 3 different material compositions. Subsequent annealing was performed at 500 °C for 24 hours under a flow of 2 vol.% H<sub>2</sub> in Ar to induce alloy formation (Pd<sub>70</sub>Au<sub>25</sub>Cu<sub>5</sub>) and to settle the microstructure (Pd). The Pt sensor was used as-fabricated, since the abundance of low index surface facets and grain-boundaries typical of e-beam evaporated metals, is beneficial for catalytic H<sub>2</sub> sensing<sup>57,90</sup>.

*Electron Microscopy:* SEM imaging was performed in a Zeiss GeminiSEM-450 at an acceleration voltage of 10.0 kV, a working distance of ca 6 mm and 200 pA beam current. EDX spectra were collected at 15 kV and 1 nA beam current using an Oxford Instrument Ultim Max 100 mm<sup>2</sup> detector. Composition quantification from the spectra was performed using Oxford Aztec 6.2.

*Data preprocessing, sequence construction and target definition for DL data analysis:* The deep-learning pipeline operated on preprocessed time-resolved optical measurements from the 64-pixel photodiode readout. For each measurement, the raw photodiode traces were baseline-corrected and normalized, after which the 64 synchronized pixel channels were assembled into temporally ordered multichannel sequences. At each time point  $t$ , the optical state of the sensor was represented as a 64-dimensional vector  $s_t$ , with channel order fixed by photodiode position. The full model input was therefore a sequence  $S = [s_1, s_2, \dots, s_T]$  in  $\mathbb{R}^{(T \times 64)}$ , where  $T$  denotes sequence length.

This representation was chosen deliberately. The 64 optical channels do not correspond to 64 physically distinct sensing materials. Instead, the seven physical nanoparticle-strip regions are optically spread and partially overlapped across the photodiode readout. The input space is therefore material-multiplexed at the hardware level and optically multiplexed at the readout level, such that each material contributes to a reproducible subset of the 64 optical features. In practical terms, this creates a structured set of partially overlapping virtual material features that preserves substantially more information than a reduced one-material-one-channel description.

The regression targets were the time-aligned gas concentration traces for  $H_2$ , CO,  $CO_2$  and NO. Relative humidity was recorded and used for plotting, regime definition and interpretation of the held-out measurements, but it was not supplied to the model as an input channel and was not treated as a supervised output. After preprocessing and alignment, each regime-specific dataset was represented as paired optical and target sequences  $(S, Y)$ , with  $S$  in  $\mathbb{R}^{(T \times 64)}$  and  $Y$  in  $\mathbb{R}^{(T \times 4)}$ . No manually selected strip averages, peak amplitudes, response times or other handcrafted kinetic descriptors were supplied to the model. The encoder was trained directly on the full multichannel optical time series.

For model fitting, the continuous sequences were partitioned into temporally ordered windows. In the direct measurement-training pipeline, overlapping sliding windows were used so that the model could access longer temporal context while still being optimized in minibatches. Window construction was performed on each regime-specific dataset without mixing held-out measurements into the training pool. The processed time traces used in the manuscript correspond to an effective plotted time step of approximately 9 s. This windowed representation exposes the encoder to uptake, recovery and delayed cross-sensitivity patterns over multiple successive time points, which are not available from a single instantaneous optical vector.

Two held-out evaluation regimes were defined *a priori*. In the dry regime, three artificial, pulsed gas-scheme measurements were used for fitting and a chemically distinct measurement was held out for evaluation. That held-out dry sequence terminated in a humidity excursion that was absent from the dry training data. In the simulated urban environment, two humid day-scale sequences were used for fitting

and a third humid day-scale sequence was held out for evaluation. In this second regime, humidity was present throughout both training and test, so the held-out condition probed transfer to a new humid dynamic sequence rather than exposure to humidity for the first time.

*Transformer architecture and training objective:* Gas decoding was performed with an encoder-only transformer operating on the preprocessed 64-channel optical sequences. Each 64-dimensional input vector  $s_t$  was first projected into a shared latent space by a learned linear embedding layer. Positional encoding was then added to the embedded sequence so that the model could distinguish temporal order and represent temporally directed dependencies even when similar optical states recurred at different times.

The embedded sequence was processed by stacked transformer encoder blocks composed of multi-head self-attention and position-wise feed-forward sublayers with residual connections and normalization. The purpose of self-attention in this setting was to allow the model to learn which time points and which combinations of optical features were most informative for estimating gas composition at a given position in the sequence. This is particularly important here because the relevant information is distributed jointly across time and across partially overlapping optical features: hydrogen uptake, competitive adsorption, humidity-induced modulation, contaminant cross-sensitivity and baseline drift all contribute to the measured signal in a coupled manner.

The contextualized latent representation produced by the shared encoder backbone was then read out by gas-specific regression heads that predicted the concentration time traces of  $H_2$ , CO,  $CO_2$  and NO as functions of time. These regression heads were distinct from the internal self-attention heads used inside the encoder blocks. The internal attention heads determined how information was integrated across time and across optical features, whereas the regression heads mapped the shared latent representation to the analyte-specific outputs. This multi-output formulation is important because  $H_2$ , CO,  $CO_2$  and NO modify the same optical readout through coupled adsorption and interference effects; the shared encoder therefore learns a common gas/sensor state before the analyte-specific readout.

The model was trained end-to-end with supervision applied only to the gas concentration targets. No supervision was applied to attention weights, material rankings or other interpretability quantities. The objective function was a gas-weighted regression loss over the predicted and target concentration time traces,  $L = \sum_g w_g \cdot MAE(y_g, \hat{y}_g)$  where  $g$  indexes the output gases and  $w_g$  denotes gas-specific weighting factors. In this formulation, the model was optimized to recover concentration time traces directly from the multiplexed optical sequences, and any subsequent attention structure used for interpretation emerged from the fitted model rather than being imposed during training.

This formulation was selected because it allows the model to exploit two coupled levels of structure simultaneously: material multiplexing in the physical chip layout and optical multiplexing in the 64-pixel readout. The methodological novelty therefore does not lie simply in applying a transformer to a sensing problem, but in using a transformer to decode a temporally evolving, optically mixed representation of a material-multiplexed sensing architecture.

*Held-out split design, baselines and validation:* Model fitting was carried out strictly on the predefined training measurements for each regime, and the held-out measurement was excluded until final evaluation. Validation was defined temporally rather than by random row sampling: the final 10% of each training measurement segment was withheld for validation, so that model selection was based on contiguous future segments rather than isolated points drawn from the same local temporal neighborhood as the training samples. This reduced temporal leakage and kept the validation problem closer to the held-out prediction setting.

The main transformer encoder was compared against three baseline model families evaluated on the same train/validation/test partitions and target time traces. The first baseline was a static ridge regressor operating on the instantaneous 64-channel optical vector  $s_t$ , thereby testing whether the gas concentrations could be decoded without explicit temporal context. The second baseline was a lagged ridge regressor operating on temporally concatenated optical features, thereby providing a linear temporal reference model with finite memory. The third baseline was a two-layer gated recurrent unit

(GRU) network with 128 hidden units and 0.1 dropout, included as a simple nonlinear recurrent comparator.

For the temporal baselines, context length was selected over 5, 11, 21 and 41 plotted time steps using only the training measurements. Ridge regularization was swept from  $10^{-3}$  to  $10^3$ . The GRU was trained for up to 30 epochs with Adam, learning rate  $10^{-3}$ , batch size 64, and early stopping patience 5, and results were summarized across three random seeds where applicable. Inputs were standardized using training data only, and the held-out measurement remained untouched until final evaluation. These baselines were included as structured comparators for instantaneous decoding, linear temporal decoding and simple recurrent decoding, rather than as an exhaustive search over all possible sequence-model families.

*Attention aggregation and performance metrics:* After training, the model was evaluated on the held-out measurement for each regime by generating full predicted concentration time traces for H<sub>2</sub>, CO, CO<sub>2</sub> and NO across the complete sequence. For each gas channel, predictive performance was quantified using mean absolute error, root-mean-square error and Pearson correlation relative to the prescribed target time trace. For H<sub>2</sub>, additional performance summaries were computed using plateau-conditioned segments obtained by excluding  $\pm 60$  s around setpoint transitions and requiring at least 120 s of stable duration, together with threshold-based metrics at 0.5, 1, 2 and 4 vol%.

For interpretability, attention was extracted during inference from the same forward pass used to generate the predicted time traces. Because the 64 optical input channels had a fixed correspondence to spatial regions of the chip, feature-wise attention could be summarized over predefined channel groups corresponding to each material region. Grouped attention maps were obtained by summing attention contributions within the fixed feature blocks associated with the same material group and then averaging over time or visualizing them as time-resolved maps, depending on the analysis.

These grouped attention summaries were interpreted as descriptive measures of model reliance and proxy observables of adsorption kinetics and causal materials ranking. Their function in the present

study was to relate the learned spatiotemporal decoding behaviour back to physically defined material regions of the sensor while remaining highly interpretable.

### **Data availability**

All data supporting the findings of this study are available in the main text and supplementary information. Source data used throughout this work (including the data used in the ML model) are available via Zenodo at <https://zenodo.org/records/21027810> (ref.<sup>91</sup>).

### **Code availability**

Information and directions to Github regarding the code utilized in this study, for the Multiplexed ML model is available via Zenodo at <https://zenodo.org/records/21027810> (ref.<sup>91</sup>).

### **Author contributions**

H.K.M. has designed, structured and trained the DL model including preprocessing of the data. S.N. and C.L. have designed and S.N. has built the sensor device. A.T., C.A., S.N and C.L. have designed the sensor chips. S.N., A.T. and J.F. have nanofabricated the sensor chips. C.A., A.T., H.K.M. and C.L. have planned the experiments. A.T. and C.A. have performed the measurements. H.K.M., S.N., P.E. and C.L. coined the initial idea. C.L. has coordinated the project. P.E. and C.L. provided the funding.

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