Supplementary Information

Modulation of population density and size of silver nanoparticles embedded in bacterial cellulose via ammonia exposure: Visual detection of volatile compounds in a piece of plasmonic nanopaper

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SUPPLEMENTARY INFORMATION CONTENT

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**Figures**

**Figure S1.** TEM micrographs showing the population density of AgNPs embedded in BC without NH$_3$ vapor exposure (A-C) and after NH$_3$ vapor exposure (D-F). The population density of AgNPs at the foreground in images A-C has been estimated to be $1473 \pm 227$ AgNP $\mu$m$^{-2}$, whereas the population density of AgNPs at the foreground in images D-F is around $302 \pm 38$ AgNP $\mu$m$^{-2}$. AgNP-BC in images D-F was exposed at an initial vapor rate of around $\sim1.2$ $\mu$g s$^{-1}$ for 12 hours. TEM micrographs were analysed via image processing through ImageJ 1.48v (Wayne Rasband, National Institutes of Health, Bethesda, MD) in order to estimate the population density of nanoparticles embedded in the BC-based composite.
Figure S2. SEM micrographs of AgNP-BC without NH$_3$ vapor exposure (A) and after NH$_3$ vapor exposure (B). No damage or structural changes were observed in the nanofibers.

Figure S3. Calibration curves displaying changes in optical density depending on the initial evaporation rate and the exposure time. The error bars represent the standard deviation of three parallel experiments.
Estimation of Evaporation rates and Limits of Detection

The evaporation rate was estimated via the computations suggested by the National Ocean Service, (2013, National Oceanic and Atmospheric Administration, http://goo.gl/ebOf2T), which are based on the model proposed by Kawamura and Mackay.¹

This estimation was carried out considering a negligible wind speed of 1 \( \mu \text{m s}^{-1} \), an ammonia concentration of 30%, an ambient temperature of 25 °C and measuring the dimensions of the drops belonging to the respective studied volumes after being deposited onto the bottom of the kind of container employed throughout this research, see details in Table S1 below.

<table>
<thead>
<tr>
<th>Volume (µL)</th>
<th>Dimensions of the drop</th>
<th>Evaporation rate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Length (cm)</td>
<td>Width (cm)</td>
</tr>
<tr>
<td>5</td>
<td>0.21 ± 0.11</td>
<td>0.21 ± 0.01</td>
</tr>
<tr>
<td>10</td>
<td>0.29 ± 0.01</td>
<td>0.29 ± 0.01</td>
</tr>
<tr>
<td>20</td>
<td>0.54 ± 0.05</td>
<td>0.5 ± 0.05</td>
</tr>
<tr>
<td>50</td>
<td>0.88 ± 0.10</td>
<td>0.83 ± 0.07</td>
</tr>
<tr>
<td>100</td>
<td>1.15 ± 0.05</td>
<td>0.96 ± 0.02</td>
</tr>
<tr>
<td>250</td>
<td>1.61 ± 0.05</td>
<td>1.35 ± 0.05</td>
</tr>
<tr>
<td>500</td>
<td>2.96 ± 0.15</td>
<td>1.96 ± 0.05</td>
</tr>
<tr>
<td>750</td>
<td>3.03 ± 0.05</td>
<td>2.36 ± 0.11</td>
</tr>
<tr>
<td>1000</td>
<td>3.1 ± 0.00</td>
<td>2.71 ± 0.10</td>
</tr>
</tbody>
</table>

We utilized the formula \( \Delta OD = 1 - (A/A_0) \) to analyze the absorbance peak modulation, where \( \Delta OD \) represents the changes in optical density; \( A_0 \), the original intensity of the absorbance peak of the nanoplasmonic membrane; and \( A \) the final intensity of the absorbance peak of the nanoplasmonic membrane. \( \Delta OD \) values corresponding to the exposure to water were considered as blank values. Different limits of detection were estimated by interpolating the \( \Delta OD \) blank value plus eight times its standard deviation into the respective calibration curve, that is, according to the exposure time of the explored corrosive vapor.
These resulting interpolations are expressed in terms of µL. As the analyzed ammonia (30%) has a density of 897 µg µL⁻¹, the mass corresponding to these calculated values was estimated using this density value as a conversion factor. The limits of detection in terms of initial evaporation rate (ng s⁻¹) were obtained by interpolating the respective ΔOD values using the curves plotted in Figure S3.

Author Contributions

A. M. and E. M-N. conceived the overall concept. E. M-N., B. H. and H. G. designed the experiments. E. M-N., B. H., H. G. and A. M. analyzed the data. B. H. performed the experiments. E. M-N., wrote the manuscript with input of B.H., A. A. and A. M. E. M-N. performed the figures with input of B.H. A. M. and E. M-N. supervised the overall project.

Supplementary References