

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

Bentolhoda Heli,^{a,b} Eden Morales-Narváez,^a Hamed Golmohammadi,^c Abdellah Ajjib, and Arben Merkoçi^{a,d*}*

^{a.} Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, Barcelona, 08193, Spain.

^{b.} 3SPack, CREPEC, Département de génie chimique, Polytechnique Montréal, Montréal, Québec, Canada.

^{c.} ACECR-Production Technology Research Institute, Ahvaz, 6139684689, Iran

^{d.} ICREA – Catalan Institution for Research and Advanced Studies, Barcelona, 08010, Spain.

*arben.merkoci@icn.cat

SUPPLEMENTARY INFORMATION CONTENT

1. Supporting Figures
2. Estimation of Evaporation Rates and Limits of Detection
3. Author contributions
4. Supplementary References

Figures

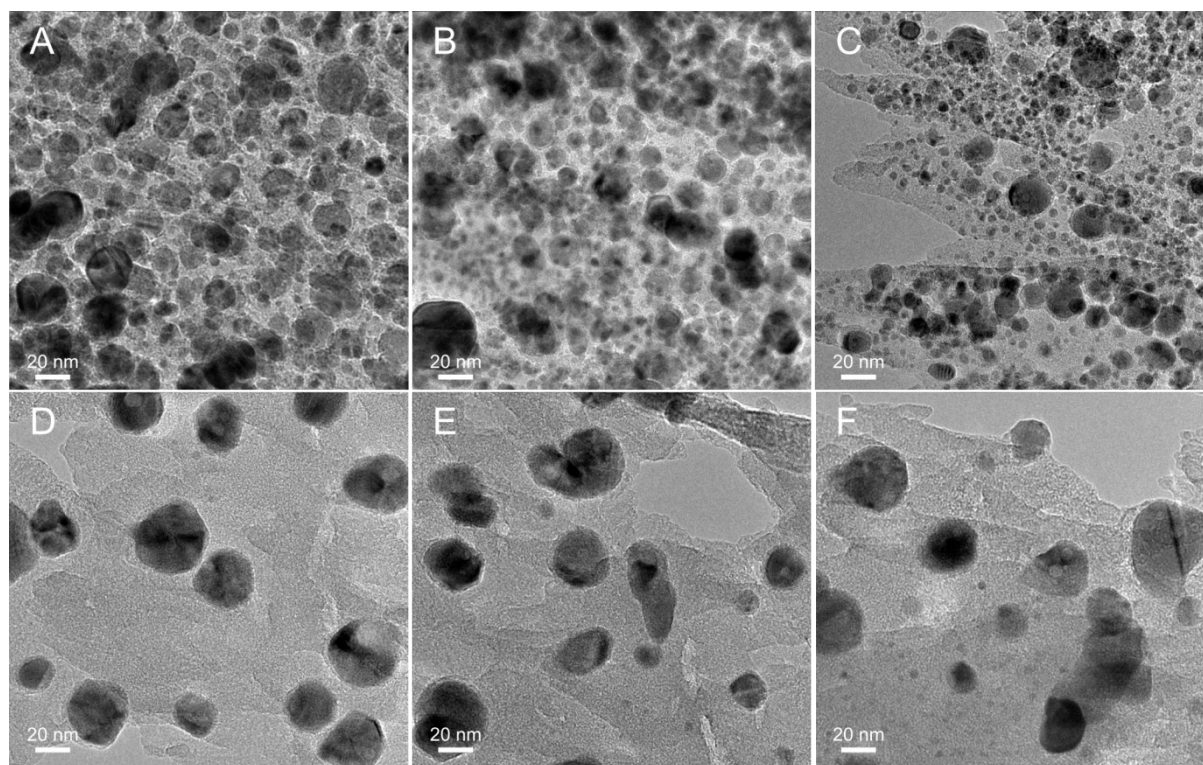


Figure S1. TEM micrographs showing the population density of AgNPs embedded in BC without NH₃ vapor exposure (A-C) and after NH₃ vapor exposure (D-F). The population density of AgNPs at the foreground in images A-C has been estimated to be 1473 ± 227 AgNP μm^{-2} , whereas the population density of AgNPs at the foreground in images D-F is around 302 ± 38 AgNP μm^{-2} . AgNP-BC in images D-F was exposed at an initial vapor rate of around $\sim 1.2 \mu\text{g s}^{-1}$ 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.

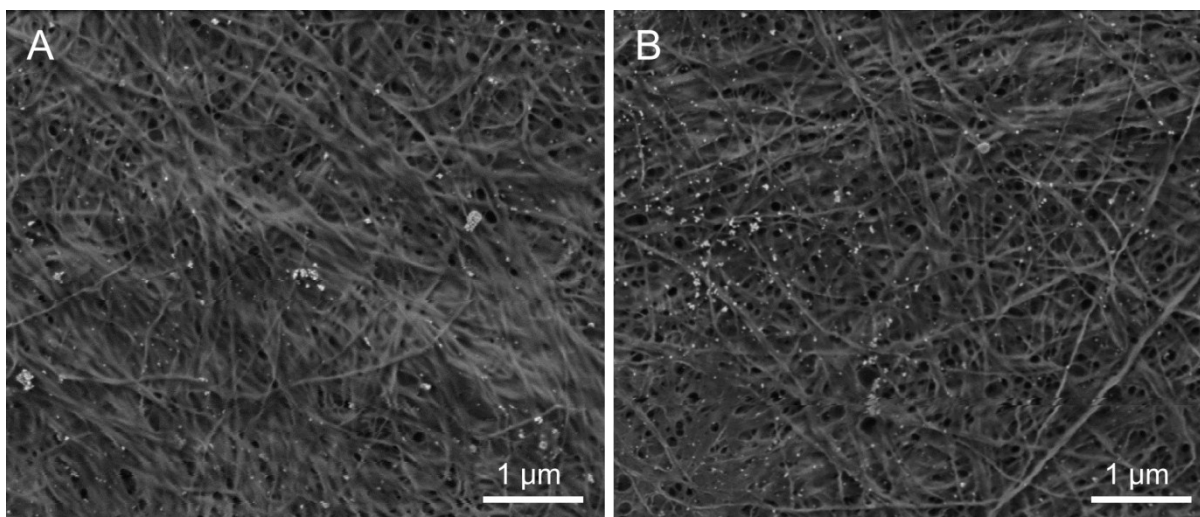


Figure S2. SEM micrographs of AgNP-BC without NH₃ vapor exposure (A) and after NH₃ vapor exposure (B). No damage or structural changes were observed in the nanofibers.

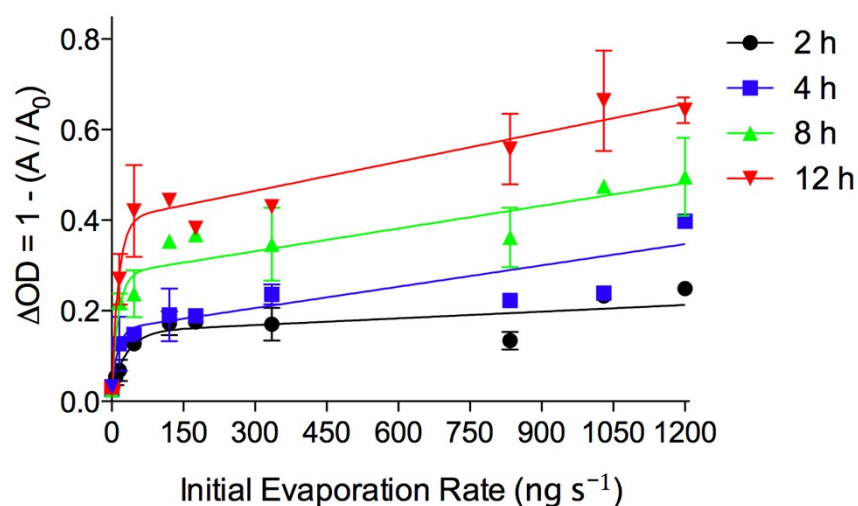


Figure S3. Calibration curves displaying changes in optical density depending on the initial evaporation rate and the exposure time. The error bars represent the standard deviation of three parallel experiments

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 S1. Estimation of initial evaporation rate of NH_3 .

Volume (μL)	Dimensions of the drop		Evaporation rate	
	Length (cm)	Width (cm)	(ng s^{-1})	($\mu\text{g h}^{-1}$)
5	0.21 ± 0.11	0.21 ± 0.01	8.51	30.6
10	0.29 ± 0.01	0.29 ± 0.01	15.7	56.5
20	0.54 ± 0.05	0.5 ± 0.05	46.9	168.8
50	0.88 ± 0.10	0.83 ± 0.07	121.0	435.6
100	1.15 ± 0.05	0.96 ± 0.02	176.0	633.6
250	1.61 ± 0.05	1.35 ± 0.05	335.0	1206.0
500	2.96 ± 0.15	1.96 ± 0.05	834.0	3002.4
750	3.03 ± 0.05	2.36 ± 0.11	1030.0	3708.0
1000	3.1 ± 0.00	2.71 ± 0.10	1200.0	4320.0

We utilized the formula $\Delta OD = 1 - (A/A_0)$ to analyze the absorbance peak modulation, where ΔOD 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. ΔOD values corresponding to the exposure to water were considered as blank values. Different limits of detection were estimated by interpolating the ΔOD 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 $897 \mu\text{g } \mu\text{L}^{-1}$, 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

1. P. I. Kawamura and D. Mackay, *J. Hazard. Mater.*, 1987, **15**, 343–364.