catalysts

MDPI

Supplementary Materials

Shape-Dependent Catalytic Activity of Gold and Bimetallic Nanoparticles in the Reduction of Methylene Blue by Sodium Borohydride

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Calculation of particle concentration and catalyst surface area from UV/Vis measurements

$$N\,[\mathrm{AuNPs\,ml^{-1}}] = \frac{\mathrm{dilution\,factor} \times \mathrm{OD}_{400} \times \left(\frac{0.0005\,\mathrm{M\,Au_0}}{1.2} \times 0.001 \right)}{\left(\frac{V_{\mathrm{AuNP}}\,[\mathrm{cm^3}] \times \rho_{\mathrm{Au}}\,[\mathrm{g\,cm^{-3}}]}{M_{\mathrm{Au}}\,[\mathrm{g\,mol^{-1}}]} \right)} \quad \text{(S1)}$$

$$S\,[\mathrm{nm^2\,ml^{-1}}] = S_{\mathrm{AuNP}}\,[\mathrm{nm^2}] \times N\,[\mathrm{AuNP\ ml^{-1}}] \quad \text{(S2)}$$

For the calculations of the particle number per ml Equation (S1) of the nanorods, the particle volume V_{Au} was obtained after measuring the SEM image (Figure 1) and dividing the gold nanorods into sections of a cylinder of 21 nm height and two hemispheres of radius 4.05 nm. In case of the bimetallic nanorods, the layer of the second metal is neglected, as the quantity is rather low and the layer is only thin. The volume of the gold-platinum nanorods was calculated likewise (cylinder of 89 nm and two hemispheres of radius 10 nm), whereas the gold-palladium nanorods were regarded as square cuboids with a height of 103 nm and square edge lengths of 18.6 nm. The surface areas were calculated based on the same principle. Furthermore, the density of gold ρ_{Au} = 19.3 g cm^{-3}, and the molar mass of gold M_{Au} = 196.97 g mol^{-1}, a dilution factor of 1, and the finding of the authors that at an optical density around OD = 1.2, a molar mass concentration of c = 0.0005 M of elemental gold is given was overall used for calculations.

Conditions and parameters used for the differential centrifugal sedimentation

DCS measurements were performed at 20000 rpm in a gradient of 11.2 ml sucrose solutions from 24%w/w to 8%w/w topped with 1 ml of tetradecane. Prior to each measurement, an external calibration was performed using an injection of 100 µl NIST-traceable standard of PVC particles with 263 nm diameter. 100 µl sample was used to run a measurement. The measurements were terminated at earliest, when a stokes equivalent diameter of 10 nm was reached or after the absorption returned to the baseline.

Set Parameters: Maximum diameter: 0.2 microns; minimum diameter: 0.002 microns; particle density: 19.32 g/ml; particle refractive index: 1.3148; particle absorption: 1 K; non-

sphericity factor: 1. Fluid density: 1.045 g/ml; fluid refractive index: 1.345; fluid viscosity: 1.07 cps.

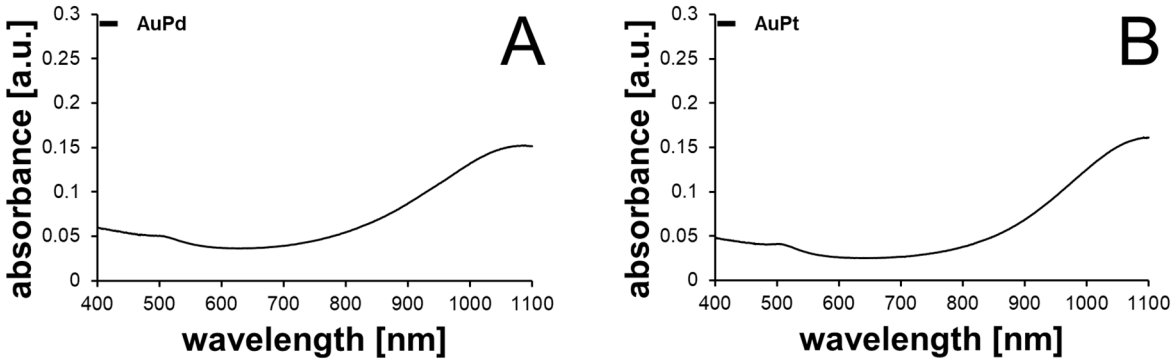


Figure S1. Original absorption spectra of AuPd- and AuPt-nanorods with dilution in water Ψ = 1:10 (A = AuPd nanorods, B = AuPt nanorods).

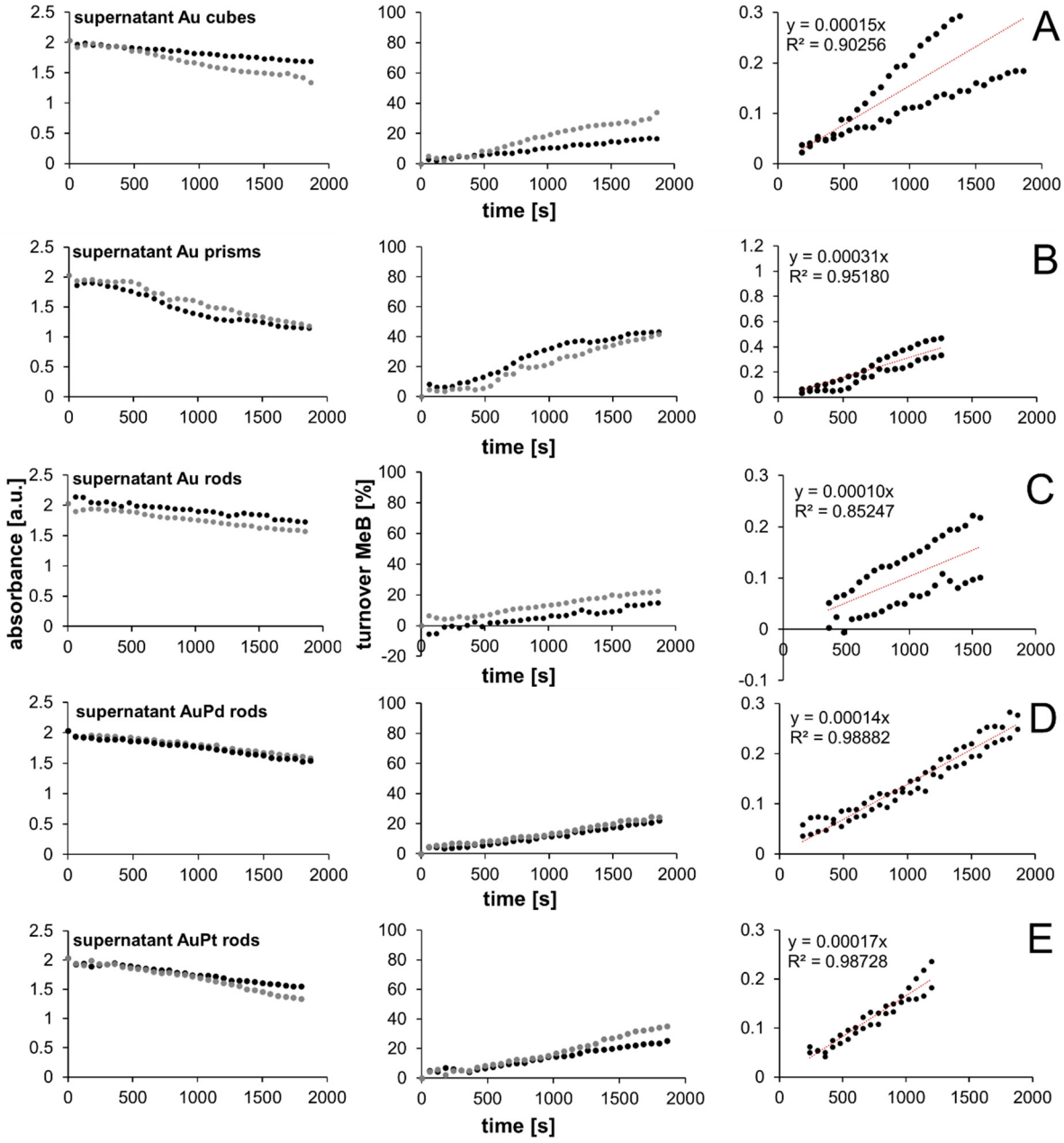


Figure S2. Development of absorbance (**left**) and MeB turnover (**middle**) and logarithmic plot of quotient of final and starting concentration over time (**right**) for the MeB reduction with different particle solution supernatants as reference (A = supernatant Au cubes, B = Au prisms, C = Au rods, D = AuPd rods, E = AuPt rods).

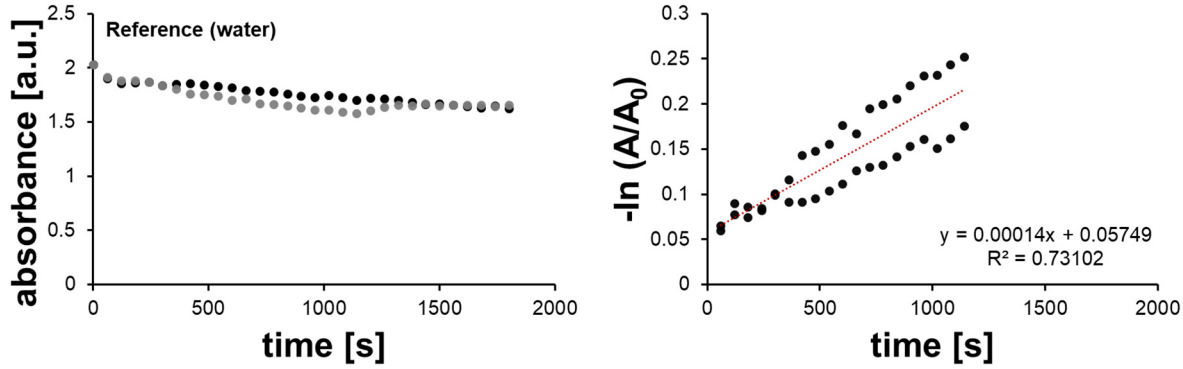
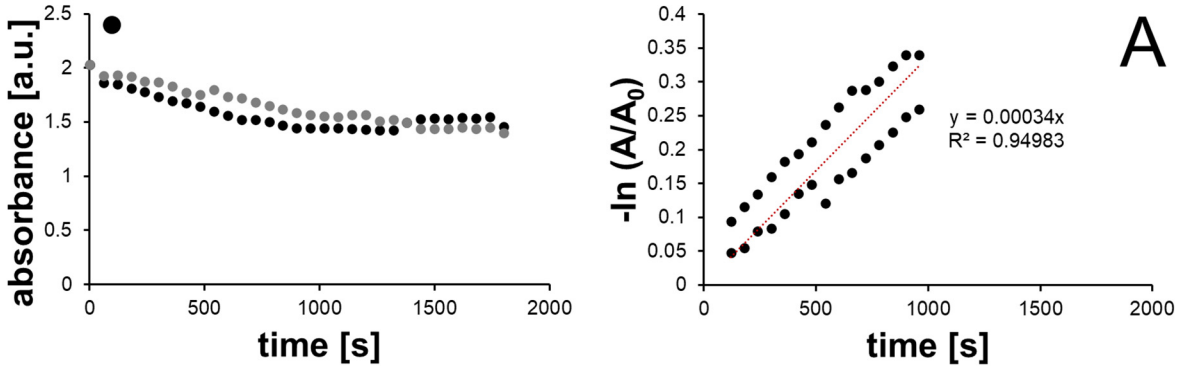
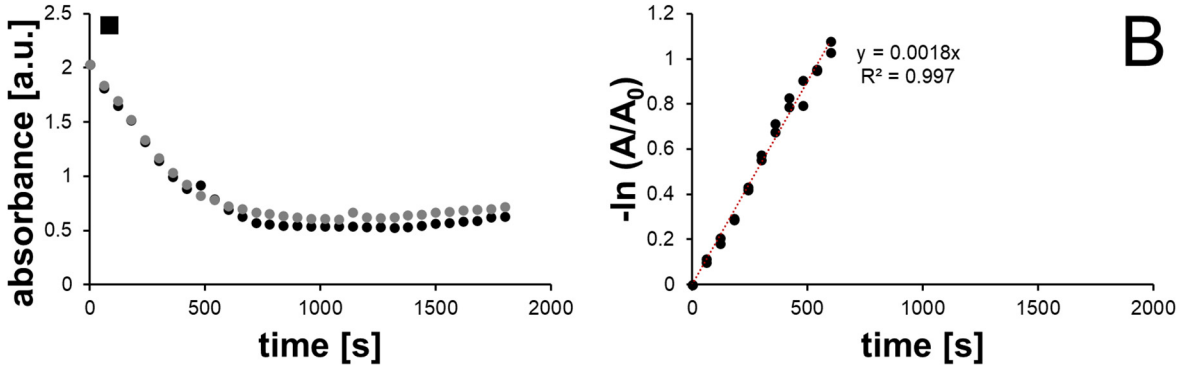


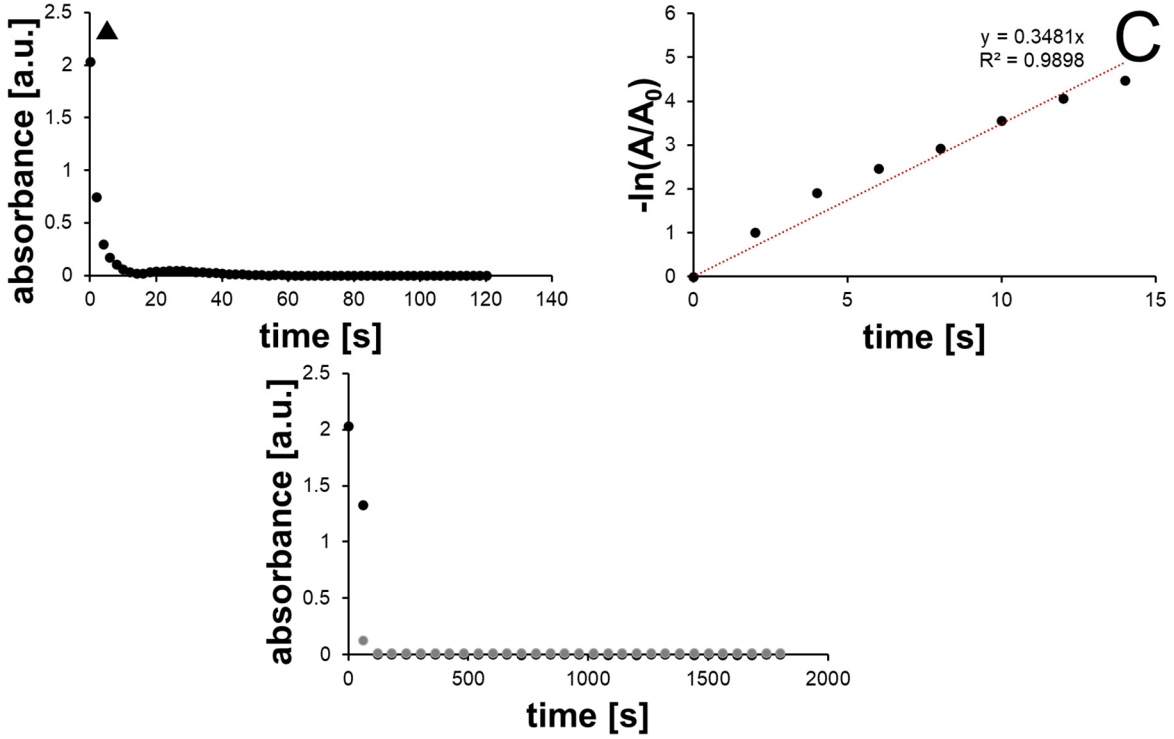
Figure S3. Development of absorbance (**left**) and logarithmic plot of quotient of final and starting absorbance over time (**right**) for the MeB reduction with water as reference.



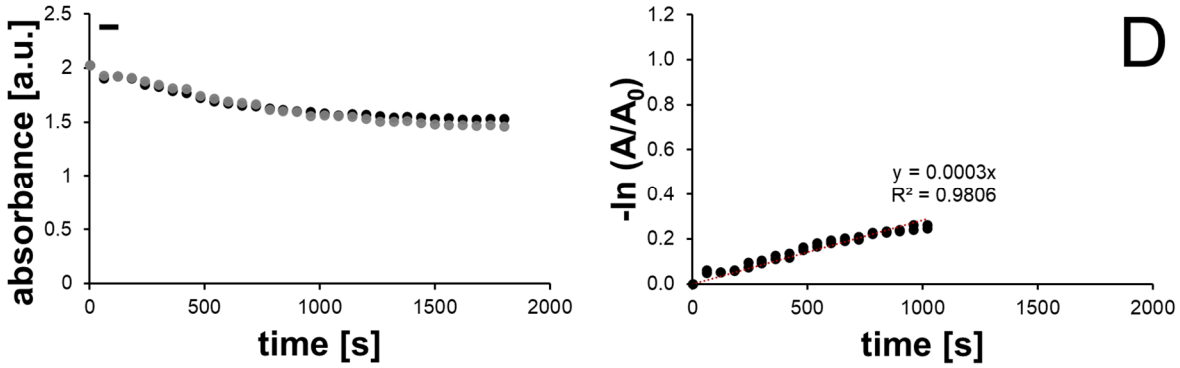
(A)



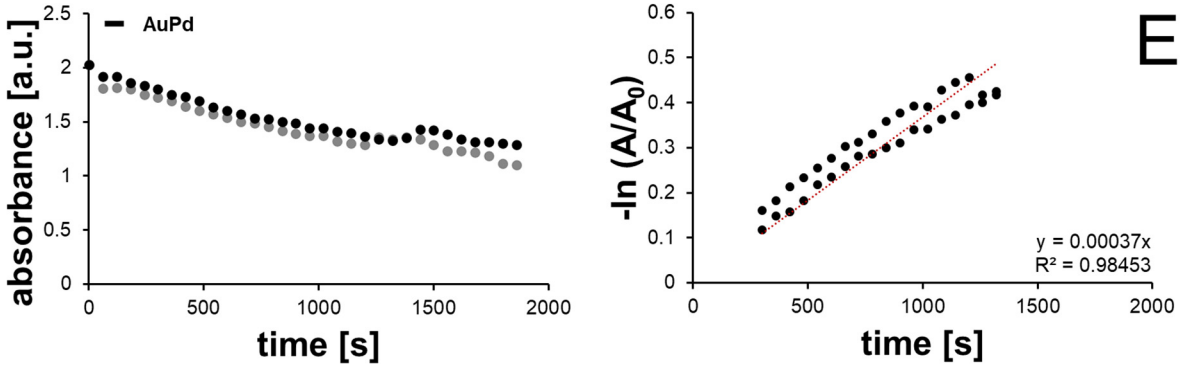
(B)


absorbance [a.u.]
time [s]
-ln(A/A0)
y = 0.3481x
R² = 0.9898
C

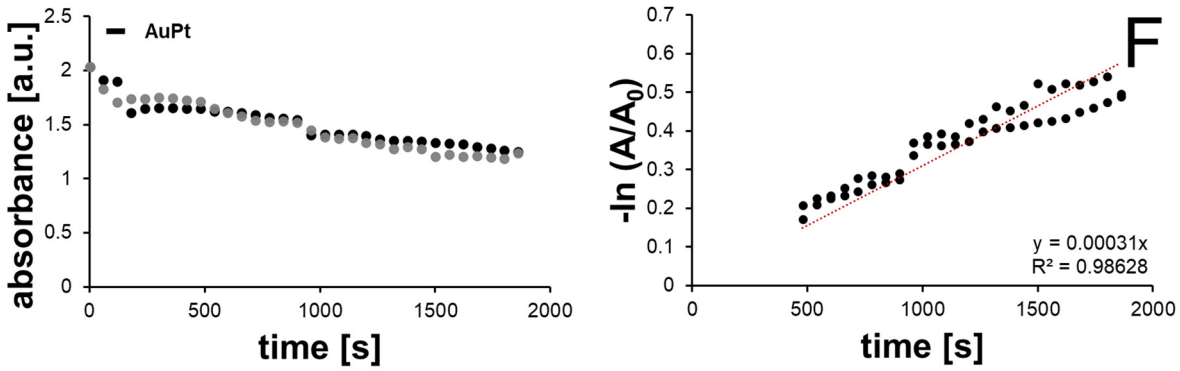
(C)


absorbance [a.u.]
time [s]
-ln (A/A0)
y = 0.0003x
R² = 0.9806
D

(D)


AuPd
absorbance [a.u.]
time [s]
-ln (A/A0)
y = 0.00037x
R² = 0.98453
E

(E)



(F)

Figure S4. Development of absorbance at λ = 665 nm (**left**) and logarithmic plot of the quotient of concentration at t and initial absorbance over time (**right**) for the MeB reduction with different particle solutions as catalysts (from top to bottom, A = gold nanospheres, B = -cubes, C = -prisms, D = -rods, E = AuPd nanorods and F = AuPt nanorods).

Table S1. Optical density of particle solutions at λ = 400 nm, number of particles per ml and available surface area per ml as calculated from Equations S1 and S2 and particle numbers obtained from differential centrifugal sedimentation measurements.

Sample	**OD400**	**$N_{UV/Vis}$ [10^{11} AuNPs ml^{-1}]**	**S [10^{14} nm^2 ml^{-1}]**	**N_{DCS} [10^{11} AuNPs ml^{-1}]**
Au nanospheres	0.543	2.24	5.13	2.12
Au nanocubes	0.412	2.54	2.56	0.68
Au nanoprisms	0.619	19.4	15.8	6.48
Au nanorods	0.948	29.6	21.9	22.4
AuPd nanorods	1.14	1.36	8.23	2.71
AuPt nanorods	1.25	1.65	11.3	1.68