

# Supporting Information

## On the Origin of Controlled Anisotropic Growth of Monodisperse Gold Nanobipyramids

Santosh Kumar Meena,<sup>\*,†,‡</sup> Frederic Lerouge,<sup>‡</sup> Patrice Baldeck,<sup>‡</sup> Chantal Andraud,<sup>‡</sup> Marco Garavelli,<sup>¶</sup> Stephane Parola,<sup>‡</sup> Marialore Sulpizi,<sup>\*,§</sup> and Ivan Rivalta<sup>\*,‡,¶</sup>

<sup>†</sup>*Chemical Engineering and Process Development Division, CSIR-National Chemical Laboratory (NCL), Dr. HomiBhabha Road, Pune-411008, India*

<sup>‡</sup>*Univ Lyon, Ens de Lyon, CNRS UMR 5182, Université Claude Bernard Lyon 1, Laboratoire de Chimie, F69342, Lyon, France*

<sup>¶</sup>*Dipartimento di Chimica Industriale "Toso Montanari", Università degli Studi di Bologna, Viale del Risorgimento 4, I-40136 Bologna, Italy*

<sup>§</sup>*Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55099 Mainz, Germany*

E-mail: sk.meena@ncl.res.in; sulpizi@uni-mainz.de; ivan.rivalta@ens-lyon.fr

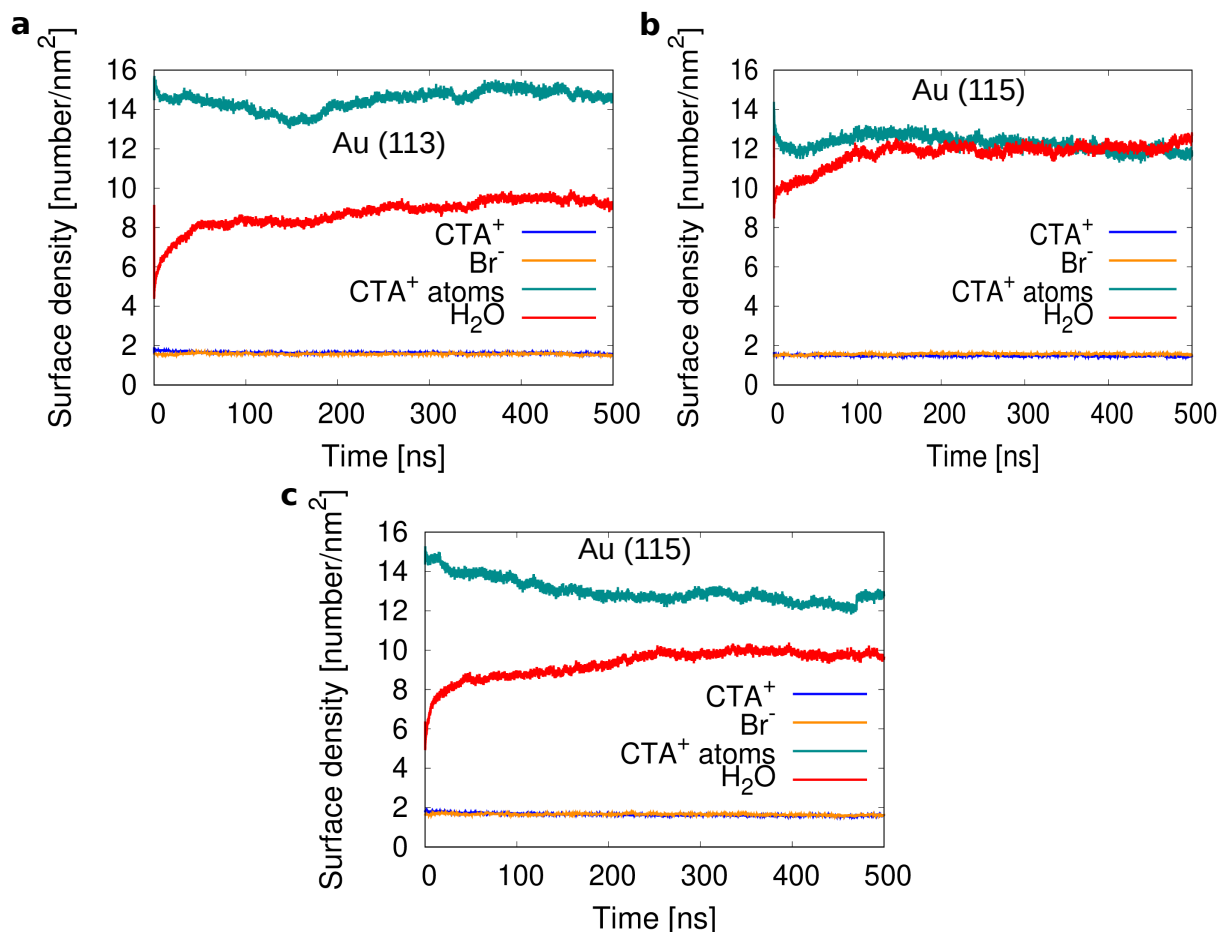


Figure S1: Average surface densities of  $\text{CTA}^+$ ,  $\text{Br}^-$ ,  $\text{CTA}^+$  atoms and  $\text{H}_2\text{O}$  represented as function of time for (a) Au(113), (b) Au(115) and (c) Au(117) as a function of time. The surface densities are average from three independent simulation runs for each surface as a function of time. The average surface densities from last 100 ns are reported in Table 2 of the main text. The surface densities are calculated based on the criteria described in ref.<sup>1</sup>

Surface densities of  $\text{CTA}^+$ ,  $\text{Br}^-$  and  $\text{Ag}^+$  on different facets of nanograin in presence of silver ( $\text{AgBr}$ ) salt are reported in Table S1. Overall surface densities of ions (sum of surface density of all the ions) on different facets of nanograin in the absence and presence of silver ( $\text{AgBr}$ ) salt are reported in Table S2.

## References

- (1) Meena, S. K.; Sulpizi, M. From gold nanoseeds to nanorods: The microscopic origin of the anisotropic growth. *Angew. Chem. Int. Ed.* **2016**, *55* (39), 11960–11964.

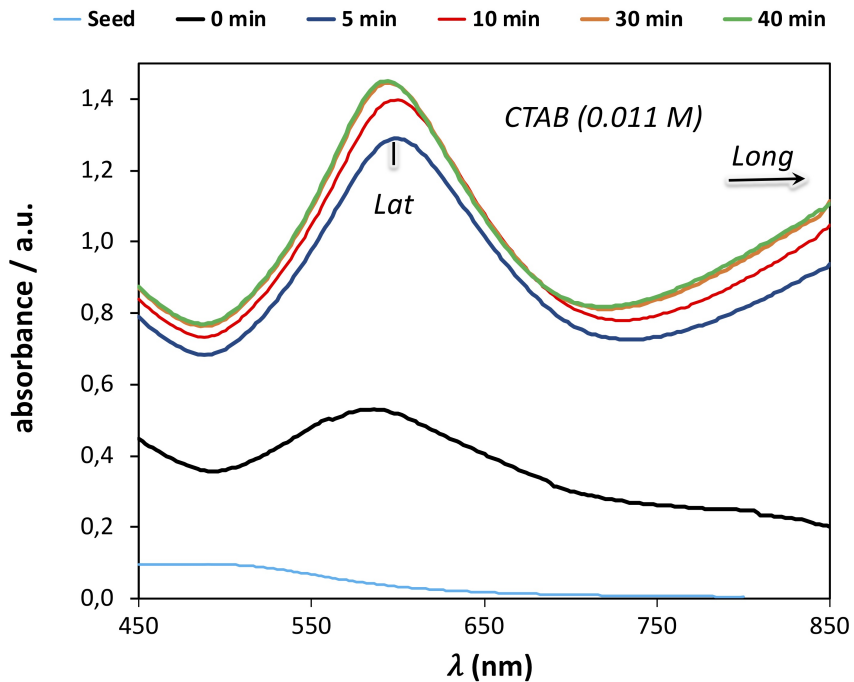


Figure S2: UV-vis spectra following the growth of the GNBs with low CTAB concentration, namely 0.01 M. Lateral (Lat) and longitudinal (Long) LSPR bands of elongated objects are indicated.

Table S1: Surface density of  $\text{CTA}^+$ ,  $\text{Br}^-$  and  $\text{Ag}^+$  on different facets of nanograin in presence of silver (AgBr) salt. The standard error is given in small brackets.

Name of surface	$\text{CTA}^+ / \text{nm}^2$	$\text{Br}^- / \text{nm}^2$	$\text{Ag}^+ / \text{nm}^2$
Au(110)	1.33 (0.41)	1.43 (0.50)	0.18 (0.07)
Au(111)	1.11 (0.16)	1.61 (0.16)	0.37 (0.07)
Au(112)	1.58 (0.06)	2.44 (0.08)	0.84 (0.04)
Au(100)	1.64 (0.06)	2.12 (0.06)	0.53 (0.03)

Table S2: Overall surface density of ions (sum of surface density of all the ions) on different facets of nanograin in the absence and presence of silver (AgBr) salt.

Name of surface	without AgBr ( $\text{ions}^- / \text{nm}^2$ )	with AgBr ( $\text{ions}^- / \text{nm}^2$ )
Au(110)	2.61	2.94
Au(111)	1.23	3.09
Au(112)	2.75	4.86
Au(100)	3.27	4.29