

Supporting Information

A closer look into the Ubiquitin Corona on Gold Nanoparticle by computational studies

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S.1 Corona thickness

Corona thickness is obtained calculating the distance between the outer beads of bounded Ubqs with the AuNP surface. The calculation was carried out for each AuNP diameter and for each model, see Fig S.1. Each layer is about 2nm thick, a value very close to Ubq diameter and it is independent on the NP size. Therefore, by using 48 molecules of ubiquitin a single layer of Ubqs is found and no evidence of more than one layer is found changing the AuNP diameter or the AuNP model.

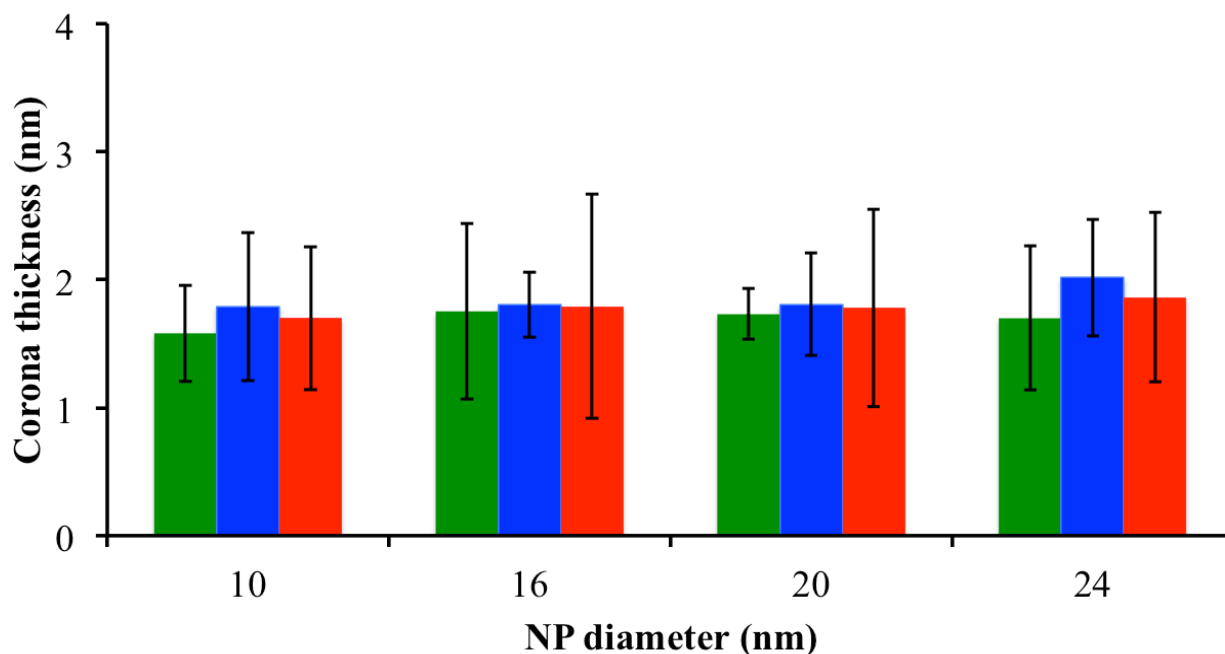


Fig S.1 Corona thickness and relative errors as a function of the NP size. In green data for the bare AuNP, in blue for the NP with implicit citrates and in red for NP with explicit citrates.

S.2 Nanoparticle adsorption capacity

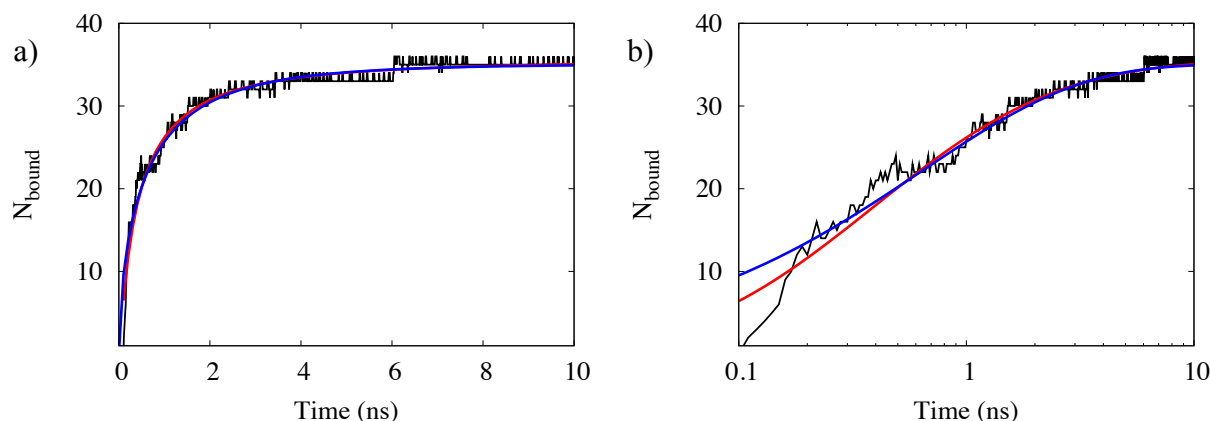


Fig S.2 Number of bonded Ubqs during simulation time, in black; the blue and red lines correspond to the fitting by the stretched-potential equation (eq. 6 in the main text), and the cumulative log-normal (eq.7 in the main text). In a) data are reported in a linear-linear scale and in b) in a log-linear scale.

S.2.1 Stretched exponential parameter

The stretched exponential values, α , obtained for the computational simulations carried out are listed in Table S.2.1. Contrary to the value ($\alpha = 0.34$) estimated by Ding et al.¹ from data obtained by Discrete Molecular Dynamics, we found a stretched exponential parameter, α , very close to 1, independently from the size of the NPs and on the environmental condition. Recalling that the stretched exponential function is used to describe relaxation kinetics with high heterogeneity in relaxation time, we may ascribe the discrepancy in the results obtained to the differences in the CG approximations of the models.

The meaningless result obtained for the 10nm diameter AuNP with explicit citrates is due to the high aggregation of Ubqs during the simulation time.

Table S.2.1 Stretched exponential value (α), with relative errors, found by fitting the number of Ubq adsorbed on the AuNP during the simulation time (eq. 6, main text).

AuNP diameter	Stretched exponential parameter α		
	Bare	Implicit	Explicit
10	0.77±0.48	0.864±0.303	2.7±2.6
16	0.786±0.096	0.896±0.152	1.094±0.4
20	0.93±0.295	1.101±0.65	0.94±0.27
24	1.77±0.09	1.125±0.527	0.749±0.09

¹ F. Ding, S. Radic, P. Choudhary, R. Chen, J. M. Brown and P. Chun. *Nanoscale* 2013, **5**, 9162–9169.