

Impact of Solvent and Ligand Density on the Self-Assembly and Optical Properties of Metal Nanocrystals

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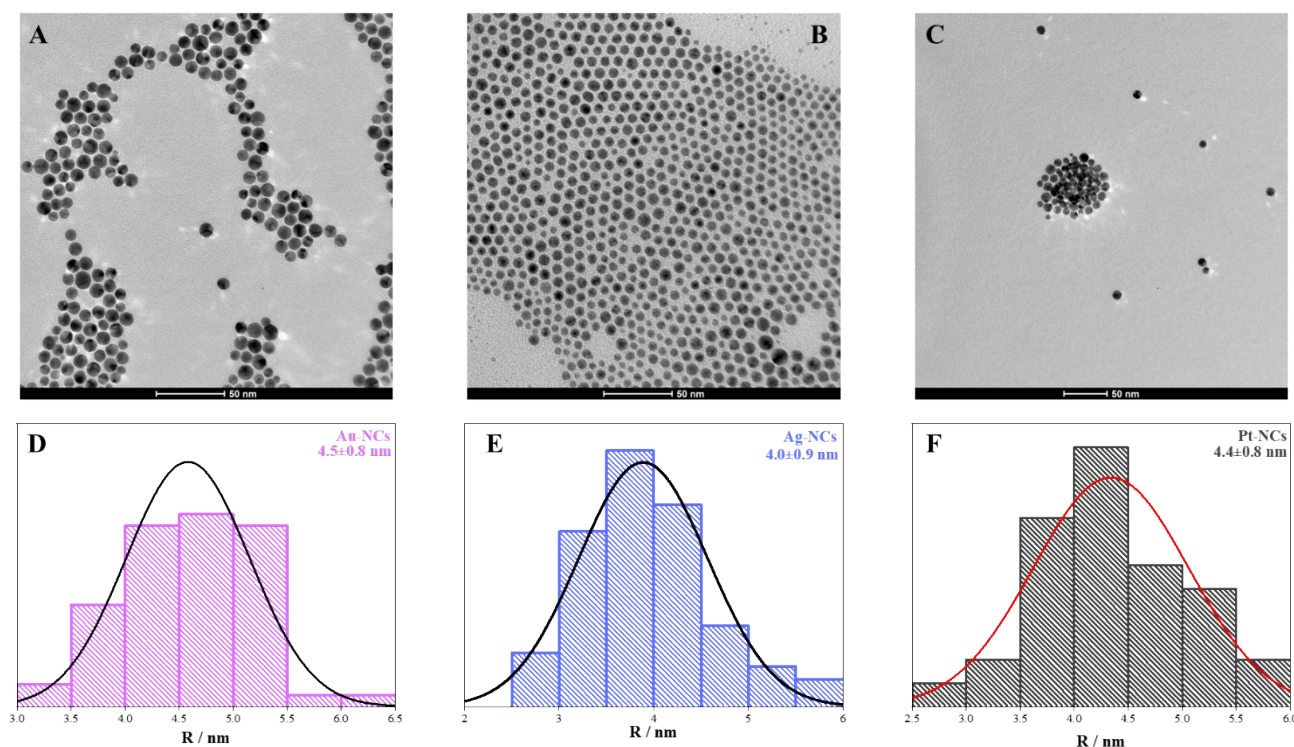
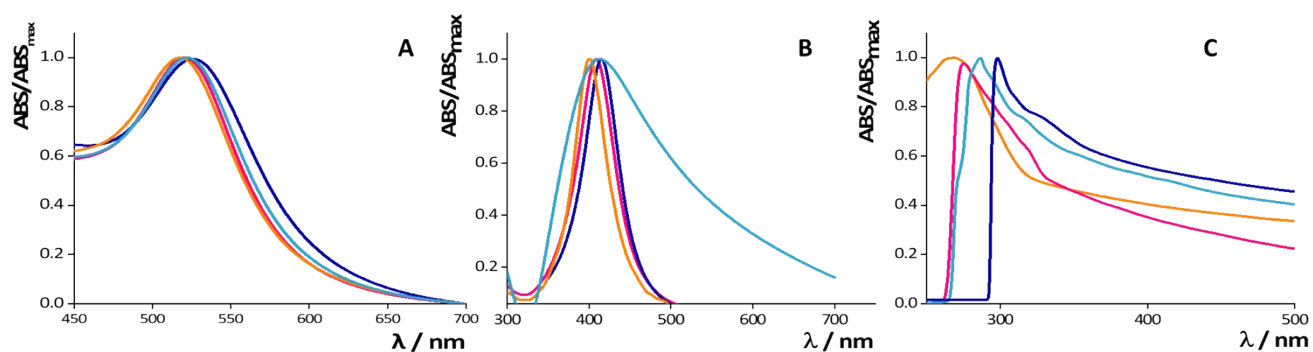


Fig. S1 TEM images of Au-NCs (A), Ag-NCs (B), and Pt-NCs (C), scale bar 50 nm; radius histogram distribution for Au-NCs (D), Ag-NCs (E), and Pt-NCs (F).

Table S1. Dielectric constant and refractive index of the selected solvents.

Solvent	Dielectric Constant / $C^2 / N\ m^2$	Refractive index
Cyclohexane	2.02	1.43
Toluene	2.38	1.49
Ethyl Ether	4.30	1.35
Chloroform	4.81	1.45

**Fig. S2** UV-Vis spectra in cyclohexane (pink line), toluene (blue line), ethyl ether (orange), and chloroform (light blue) of oleylamine-coated Au-NCs **(A)**, Ag-NCs **(B)**, and Pt-NCs **(C)**.**Table S2.** $\lambda_{\max}$ for Au-NCs, Ag-NCs, and Pt-NCs.

Solvent	Refractive index	$\lambda_{\max}$ Au-NCs / nm	$\lambda_{\max}$ Ag-NCs / nm	$\lambda_{\max}$ Pt-NCs / nm
Ethyl Ether	1.35	518	402	267
Cyclohexane	1.43	520	409	275
Chloroform	1.45	522	413	286
Toluene	1.49	526	416	297

Table S3. Peak position, Q/Q_1 ratio, and hkl indices for the C14 Frank-Kasper phase.

Sample	$Q / \text{\AA}^{-1}$	Q/Q_1	hkl
OA@Au-NCs in water functionalized from Au-NCs dispersed in cyclohexane	0.0337	1.00	100
	0.0636	1.88	103
	0.1085	3.21	205
OA@Au-NCs in water functionalized from Au-NCs dispersed in toluene	0.0333	1.00	100
	0.0622	1.88	103
	0.1068	3.21	205
OA@Ag-NCs in water functionalised from cyclohexane	0.03626	1.00	100
	0.0683	1.88	103
	0.1158	3.20	205

Table S4. Peak position, Q/Q_1 ratio, and indexing for the FCC structures

Sample	$Q / \text{\AA}^{-1}$	Q/Q_1	hkl
OA@Au-NCs in water functionalized from Au-NCs dispersed in ethyl ether	0.0569	1.00	111
	0.0652	1.15	200
	0.1178	2.08	222
	0.1599	2.82	422

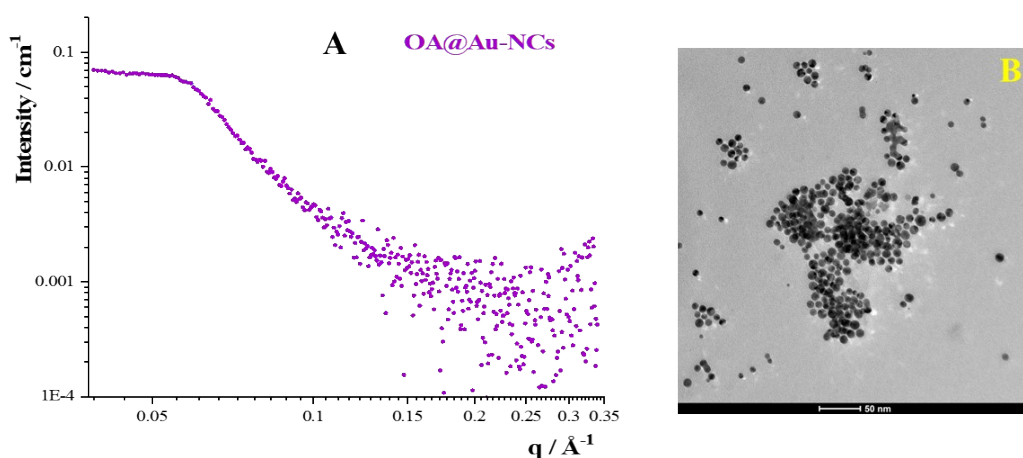


Figure S3 SAXS pattern for OA@Au-NCs in water functionalised from Au-NCs dispersed in chloroform **(A)**; TEM image of OA@Au-NCs, scale bar 50 nm **(B)**.

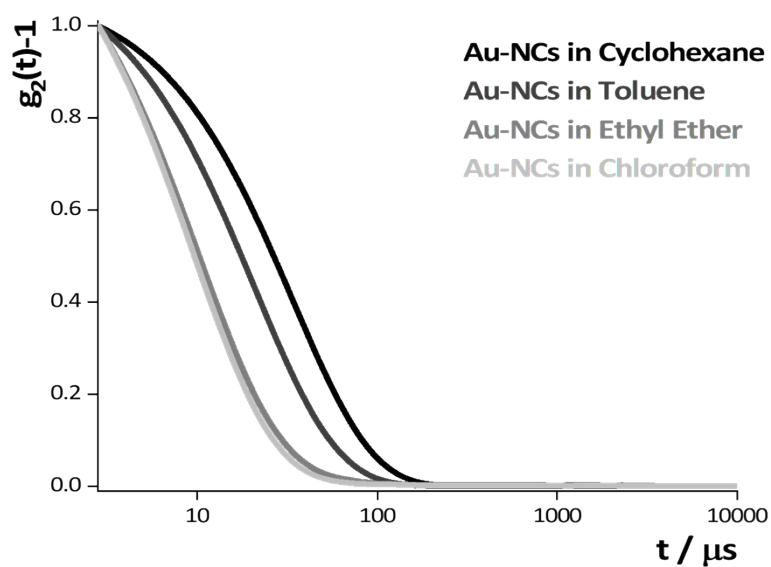


Figure S4 Correlation functions for the Au-NCs dispersed in the increasing dielectric constant solvents: cyclohexane, toluene, ethyl ether, and chloroform.

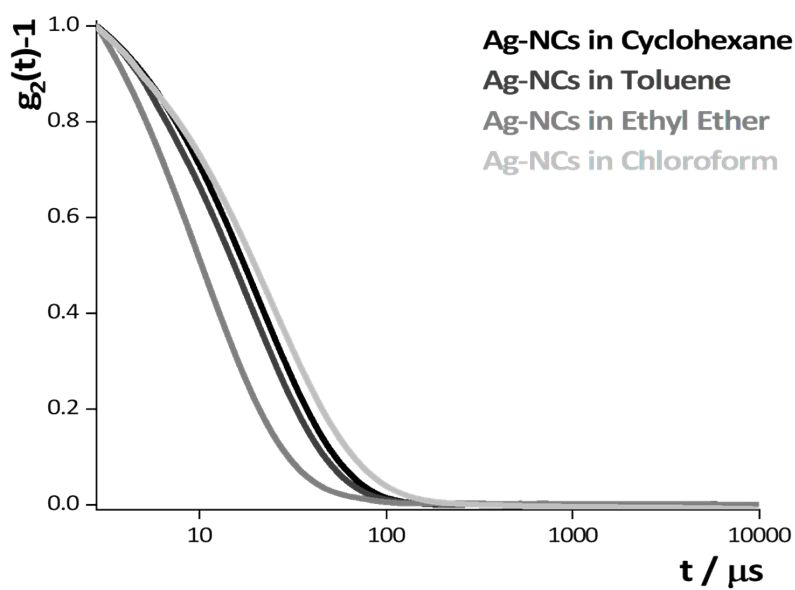


Figure S5 Correlation functions for the Ag-NCs dispersed in the increasing dielectric constant solvents: cyclohexane, toluene, ethyl ether, and chloroform.

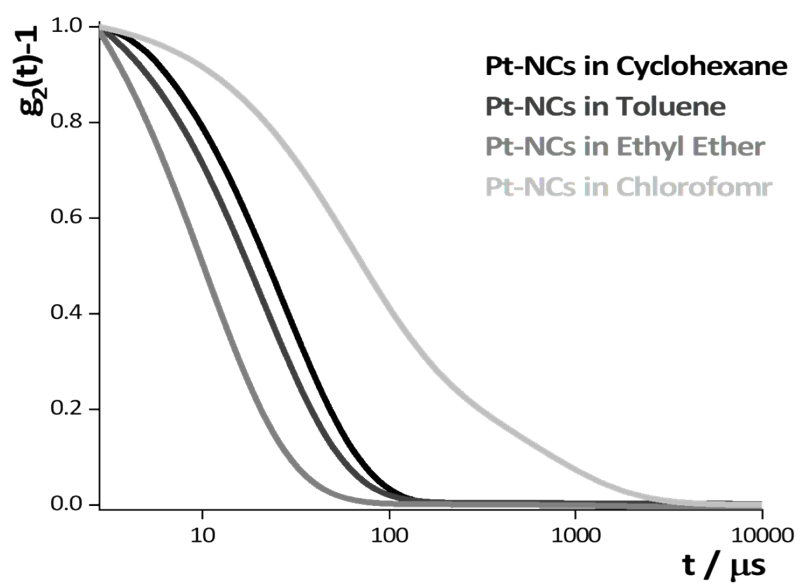


Figure S6 Correlation functions for the Pt-NCs dispersed in the increasing dielectric constant solvents: cyclohexane, toluene, ethyl ether, and chloroform.