## Supplementary information for

## Nanoparticle Translocation across the Lung Surfactant Film Regulated by

## **Grafting Polymers**

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System	Grafting	Monomer	Terminal	Surface	Repeat	Ensemble
	density	number	charge	tension	times	method
		per chain	(e)	(mN/m)		
NP+LS	20%	5	1	20	1	NVT
NP+LS	60%	5	1	20	1	NVT
NP+LS	100%	5	1	20	1	NVT
NP+LS	20%	10	1	20	1	NVT
NP+LS	60%	10	1	20	1	NVT
NP+LS	100%	10	1	20	1	NVT
NP+LS	20%	5	-1	20	1	NVT
NP+LS	60%	5	-1	20	1	NVT
NP+LS	100%	5	-1	20	3	NVT
NP+LS	20%	10	-1	20	1	NVT
NP+LS	60%	10	-1	20	1	NVT
NP+LS	100%	10	-1	20	6	NVT
NP+LS	100%	7	-1	20	1	NVT
NP+LS	100%	8	-1	20	1	NVT
NP+LS	100%	8	-1	10	1	NVT
NP+LS	100%	10	-1	10	1	NVT
NP+LS	100%	10	-1	10	1	NPT
NP+LS	100%	10	-1	40	1	NVT
NP+LS	20%	5	0	20	1	NVT
NP+LS	60%	5	0	20	1	NVT
NP+LS	100%	5	0	20	1	NVT
NP+LS	20%	10	0	20	1	NVT
NP+LS	60%	10	0	20	1	NVT
NP+LS	100%	10	0	20	6	NVT
NP+LS	100%	10	0	10	1	NVT
NP+LS	100%	10	0	10	1	NPT
NP+LS	100%	10	0	40	1	NVT
NP+lipid	100%	10	-1	20	1	NVT
NP+lipid	100%	10	1	20	1	NVT

Table S1. Summary of simulations performed and the pertinent conditions. NP+LS stands for the NP with the lung surfactant monolayer. NP+lipid stands for the NP with the lipid monolayer without proteins.



Figure S1. Dynamic Z position and final state of the negatively charged NPs (grafting with 7 and 8 monomers with grafting density of 100%).



Figure S2. Snapshots of the equilibrated states of the negatively charged and neutral NPs (grafted with chains of 8 monomers with grafting density of 100%) after interacting with the lung surfactant film.



Figure S3. The order parameter of the phospholipids of the lung surfactant film at different surface tensions. The chain order parameter was calculated using the formula:

$$Sz = \langle \frac{1}{2}(3\cos^2\theta_n - 1) \rangle$$
, which is used to reflect the phase separation of the lung

surfactant film<sup>1</sup>.  $\theta_n$  is the angle between the vector connecting the neighboring sites of the hydrocarbon chain and the monolayer normal direction.



Figure S4. The interaction energy between the neutral and negatively charged NPs and the lipids tails under different surface tensions.

1. S. Baoukina, E. Mendez-Villuendas and D. P. Tieleman, *J. Am. Chem. Soc.*, 2012, **134**, 17543-17553.