

# Supporting Information

## Conformations and effective interactions of polymer coated nanoparticles at liquid interfaces

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### S1. PARTICLES IN THE BULK

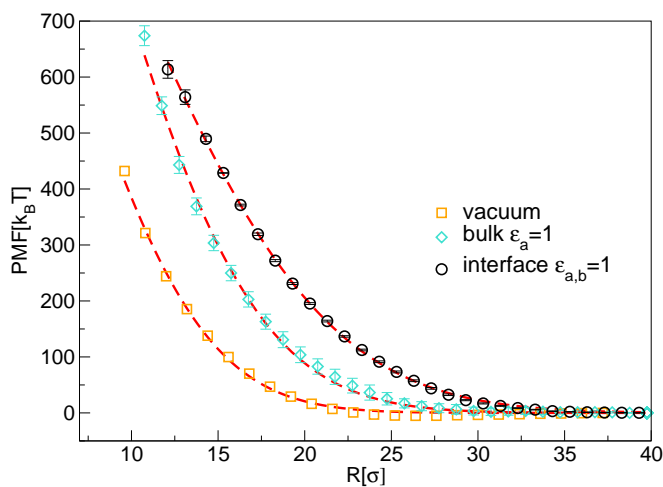


FIG. S1. Comparison of the potential of mean force for the interaction of two NPs with chain length  $L = 20$  at the interface and in the bulk ( $\epsilon_{a,b} = 1.0$  for the monomer-solvent interaction) and for NPs in “vacuum” (without explicit solvent). Note, that the distance  $R$  is defined in 2D for the particles at the interface and in 3D for the bulk systems. The red dashed lines are fits with the Gaussian  $U(R) = \epsilon_g \exp(-(R/\sigma_g)^2)$ .

The interaction between core-shell-particles in the bulk was investigated previously in simulations, but mostly without explicit solvent [1–3]. Therefore, we also want to comment on the properties of bulk systems simulated with our model. The effective interactions in bulk are shorter ranged compared to the NPs at an interface, due to the fact that the latter interact via the stretched chains at the interface (Fig. S1). Since there is no additional stretching of the chains in the first place, the chains of NPs in bulk are not as much compressed as interface systems when the NPs come closer as is displayed in Fig. S2. The stretching of chains, when they are squeezed out from between the NPs is more pronounced in the bulk,

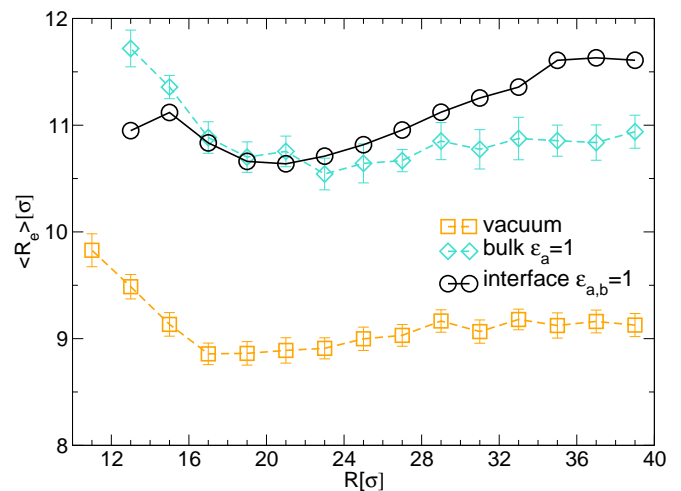


FIG. S2. End-to-end distance of the polymers ( $L = 20$ ) whose first monomer lies in the volume between the two NPs with chain length  $L = 20$  at the interface and in the bulk ( $\epsilon_{a,b} = 1.0$  for the monomer-solvent interaction) and for NPs in “vacuum”. Note, that the distance  $R$  is defined in 2D for the particles at the interface and in 3D for the bulk systems.

since the NPs can partially detach from the interface in the case of the 2-dimensional interaction.

The large difference in the PMF for the bulk systems with explicit solvent and without explicit solvent (“vacuum”) is remarkable. We observe a difference in the swelling of the polymers when the solvent molecules are explicitly taken into account. While  $R_e$  differs only by  $2\sigma$ , the range of the effective interactions is shifted by roughly  $5\sigma$ . This demonstrates that “vacuum” is not such a good solvent for our grafted polymers. And it underlines, that seemingly small differences in the average polymer conformations can have a large impact on the effective NP interactions.

## S2. ADDITIONAL DATA FOR $L = 5$

Fig. S3 and S4 show the monomer and solvent concentration and the NP-positions as a function of  $R_{2d}$  for systems with  $L = 5$  in analogy to the data for  $L = 20$  in the main article.

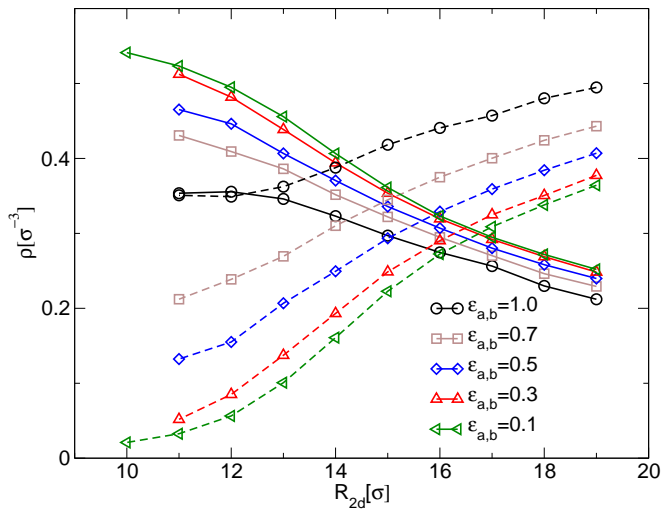


FIG. S3. Concentration of monomers (bold lines) and solvent particles (dashed lines) between the two NPs as function of the NP-distance  $R$  for different strengths  $\epsilon_{a,b}$  of the monomer-solvent interaction for systems with  $L = 5$ .

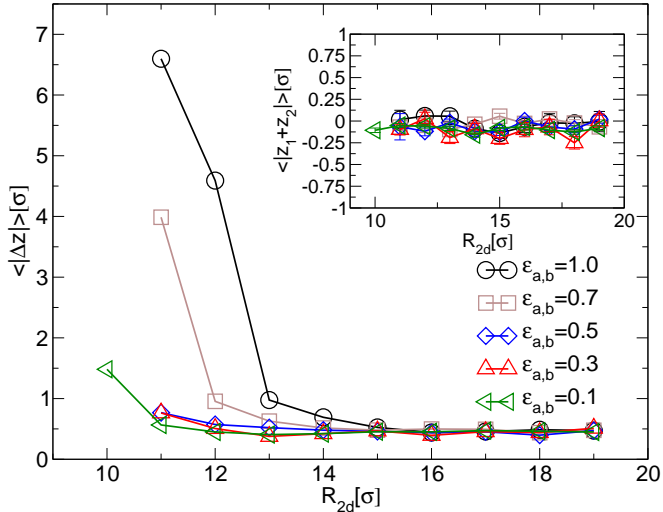


FIG. S4. Mean height difference between the two NPs as a function of their distance  $R$  for systems with  $L = 5$ . Inset: Asymmetry of particle detachment from the bulk measured by  $|z_1 + z_2|$  where  $z_1$  and  $z_2$  are the  $z$ -coordinate of the core of NP 1 and NP 2, respectively.

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