

Computer Investigation on the Influence of Chain Length on the Shielding Effect of PEGylated Nanoparticles

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1 The model of grafted nanoparticles

PEG chains were randomly linked on the surface of a naked NP core mimicking a covalently decoration of a NP in the experiments. The ratio of PEG chains to surface beads of NPs is 1:5. The end-to-end distance between the beads in two end of PEG chain was defined as the transient chain length of PEGs to measure the extending behavior of PEGs in the adsorption.

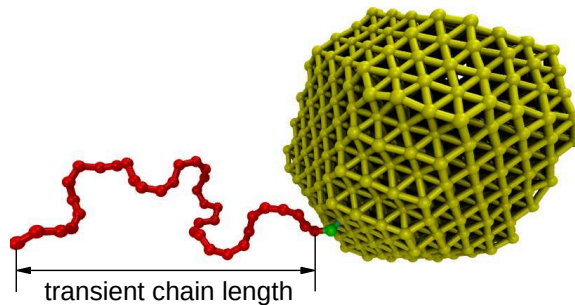


Figure 1: The model of a grafted nanoparticle. A yellow bead cluster represents a solid NP core; a red beads chain represents a grafted PEG molecule; a green bead represents the linker.

2 The recovery process of the membrane

The surface functionalization of PEGs can improve the aqueous solubility of a hydrophobic NP, thereby affecting the interaction of the nanoparticle with the biomembrane. In-

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stead of entrapping into the membrane, the PEGylated NP only adsorbed on the lipid bilayer with some small fluctuations. An artificial pulling constraint forced the PEGylated NP to move towards the membrane, enhancing the bending of the membrane. When this artificial force was revoked, the membrane restored its preceding flat state due to the wrap hindrance of PEG molecules. An animation of the recovery process is available in Supplementary Information, SI.2.

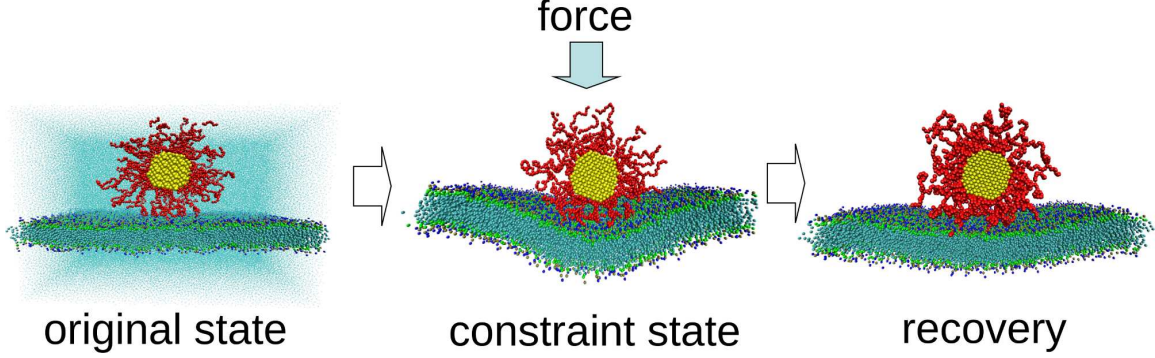


Figure 2: The recovery process of the membrane after revoking the constrained pull on the grafted nanoparticle.

3 Generating indices of PEGs on a NP10nm-PEG36

In the case of NP10nm-PEG36, there are 400 PEG36 molecules grafted on the surface of NP10nm. Firstly, as shown in Figure 3(a), we designated the PEG molecule at the bottom of the NP as the first molecule (index 1) and the PEG on the top of the NP as the last molecule (index 400). All indices of PEG molecules can be assigned along the searching path of an spherical helix curve around the NP. Then we re-arranged indices of PEGs in the manner as shown in Figure 3(b) for a more intuitive manifestation. After that, those indices of PEGs grafted at the bottom of the NP were moved to the middle position of the index array, ensuring that these variations of transient chain length of PEGs interacting with the membrane can be exhibited in the middle of Figure 7 in the manuscript. At last, we re-ordered all indices of PEGs in the manner as shown in Figure 3(c) to generate final indices for individual PEGs.

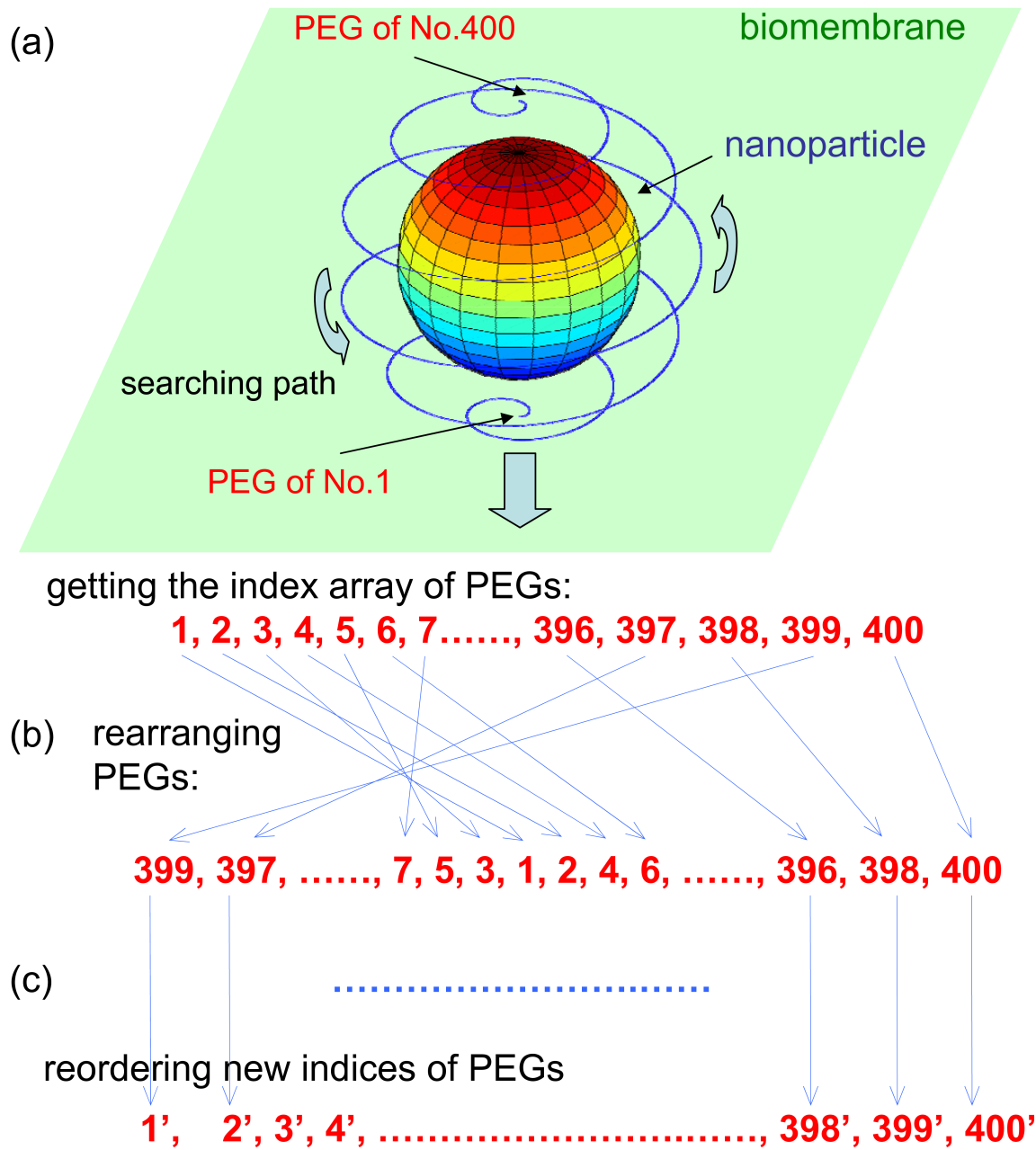


Figure 3: The generation of indices of individual PEGs: (a) getting indices of PEGs; (b) re-arranging indices of PEGs; (c) re-ordering their new indices for individual PEGs.