

Wetting behavior of PEO-grafted silica surface in presence of free homopolymers

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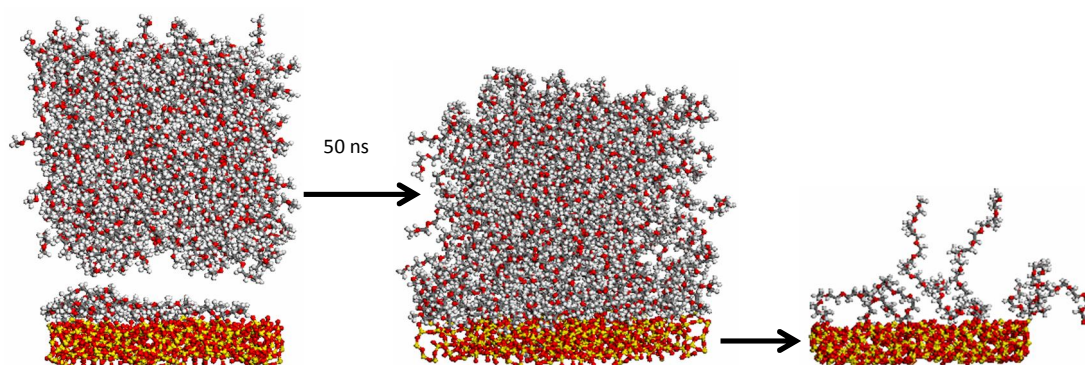
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Properties of polymer-grafted surfaces are conveniently tuneable and this approach has found a great deal of technological, biomedical or biochemical application [1]. The interactions of surfaces with a matrix of free polymer chains might be manipulated by irreversible coating of such surfaces with chemically identical polymer chains. A system composed of a single polymer-grafted surface immersed in a matrix of homopolymers is theoretically equivalent to a system of two opposing polymer-grafted surfaces, thus, the behaviour of the later system is deduced from the behaviour of the former system [2].

Atomistic molecular dynamics study has been performed to characterize the conditions at which free poly(ethylene oxide) (PEO) chains are prevented from penetration into a layer of PEO chains end-grafted on the amorphous silica surface. The grafting density of anchored PEO chains and the molar mass of free PEO chains are the variable parameters. The density distributions of free and grafted PEO chains, height of the grafted layer, overlap parameters and orientation order parameters have been calculated and analysed. The comparison with the theoretical phase diagram has been drawn. As high grafting density as ~ 3.5 chains/nm² is needed for free PEO chains to be expelled from the grafted PEO layer on the silica support. It appears that two opposing PEO-grafted surfaces would not adhere when exposed to bulk free PEO chains of comparable molar masses. Depending on the molar mass of free PEO chains the grafted layer behaves like being immersed in a good or Θ -solvent [3].



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- [1] M. Motornov, S. Minko, K.-J. Eichhorn, M. Nitschke, F. Simon and M. Stamm, *Langmuir*, 2003, **19**, 8077.
- [2] M. W. Matsen and J. M. Gardiner, *J. Chem. Phys.*, 2001, **115**, 2794.
- [3] Z. Benková and M. N. D. S. Cordeiro, *Langmuir*, 2015, **31**, 10254.