116th MSS-Seminar
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Nägelsbachstr. 49b

Theoretical and numerical analysis of polyelectrolyte-based nano-actuators

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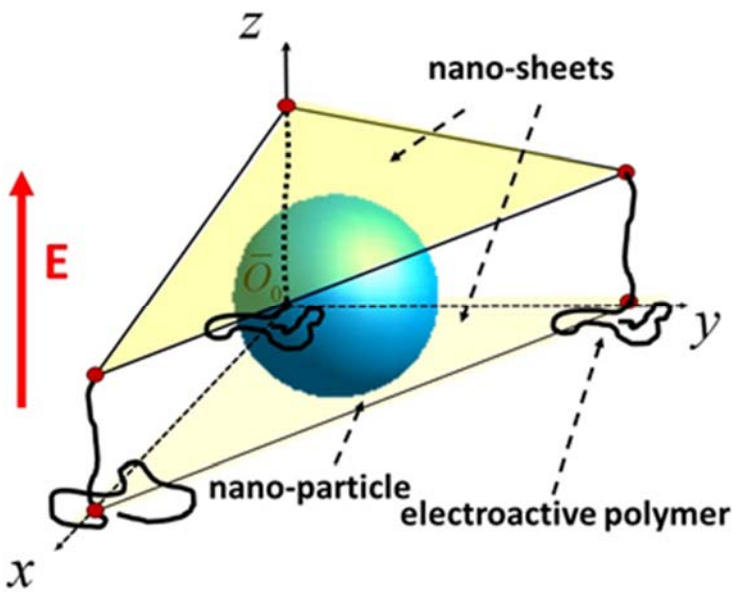

We analyse, theoretically and by means of molecular dynamics (MD) simulations, the generation of mechanical force by a polyelectrolyte (PE) chain grafted to a plane and exposed to an external electric field; the free end of the chain is linked to a deformable target body. Varying the field, one can alter the length of the non-adsorbed (bulk) part of the chain and hence the deformation of the target body and the arising force. Next, we study the effectiveness of possible PE-based nano-vices, comprised of two clenching planes connected by PEs exposed to an external electric field. We analyse a novel phenomenon – two-dimensional diffusion of a nano-particle, clenched between two planes, and introduce a quantitative criterion for clenching efficiency.

Using first a microscopic counterpart of the Coulomb friction model, and then a novel microscopic model based on surface phonons, with the vibration direction normal to the surface, we calculate the clenching coefficient as a function of the external electric field. Our results demonstrate a dramatic decrease of the diffusion coefficient of a clenched nano-particle for the range of parameters relevant for applications; this proves the effectiveness of the PE-based nano-vices.