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Transport properties of nanoparticles studied by Brownian dynamics simulations

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1. Introduction

In general, nanoparticles display irregular surface topograph. The bead models consisting of structure-less subunits are only suited for semi-quantitative analysis of nanoparticle dynamics. As a first step on the road towards quantitative modelling of nanoparticles we have introduced non-spherical subunits called nuggets.

Our Brownian dynamics (BD) analysis incorporates stretching, bending and torsional stiffness between nearest neighbor units, exluded volume effects, external force fields, fluid flow and fluiddynamic interactions.

The resulting Brownian dynamics algorithm is capable of carrying out equilibrium as well as non-equilibrium simulations for both nanoparticles in dilute solution and liquid crystals.

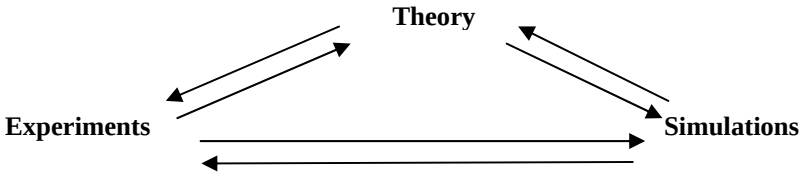

Fig. 1: Goal: A quantative Brownian dynamics analysis of nanoparticles.

2. Conclusion

By analyzing experimental data using the theory presented in this poster we can in principle determine the molecular parameters that are included in the theoretical description.

The work presented here provides several alternative approaches for modelling of polymers consisting of rigid segments. Only detailed comparison of numerical estimations and precise experimental results can tell which theoretical model is the most appropriate.

The theoretical foundation for BD-simulation of a wide class of nanoparicle chains, including segmented biopolymers, appears to have been firmly established.

References

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