Study of the anomalous translational and rotational diffusion properties of macromolecules in solution: microscopic view point.

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In this contribution we investigate the translational as well as rotational diffusion of the non—rigid macromolecules in solution by starting from the microscopic view point, i.e. when the macromolecules are described in terms of their molecular subsystems, the so- -called *beads* of the macromolecule. When immersed into a solvent, which is assumed as a set of (larger number of) particles, of course, the shape and the diffusion behaviour of a macromolecule will depend not only interaction among its individual beads but will be affected also by the surrounding particles from the solvent.

A novel, semi- -phenomenological expression is derived for the friction tensor of macromolecules immersed into solution.[1, 2] By making a few realistic assumptions about the interaction of the molecular beads with the particles of the solvent, the friction tensor is expanded into a series of terms which purely depend on the $(k+2)$- point correlation functions of the solvent as defined in the kinetic theory of the liquids. In a first application [3] of this series expansion, the boundary condition and diffusion coefficients are investigated for a single bead in dependence on the strength of the interaction among the solvent particles and with the macromolecule. When compared with previous molecular- -dynamical simulations, excellent agreement is found even for a rather strong coupling between the bead and the solvent. In addition, we also study and compare with molecular dynamic simulation works the effects of the various bead—solvent potentials on the friction tensors of macromolecule for the high density and critical solvent The results from the semi- -phenomenological theory are found to compare well with MDS works over a wide range of mass ratios and at quite different temperatures and viscosities of the solvent.[2]

In respect to the rotational motion, we consider the non—rigid macromolecule immobilized on a surface. We investigate the influence of the bead—bead as well as bead—surface interaction potentials on the orientation and relaxation processes of the biomolecules immersed in the solvent. We present and discuss the explicit expression for the configuration- -space distribution function of such molecules. Results from calculations are then compare with other computations which are based on a rigid- -rod model of the macromolecules[4].

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