Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Statics and dynamics of softly confined polymers ANDREA SCAGLIARINI, MAURO SBRAGAGLIA, Department of Physics, University of Rome "Tor Vergata", MARCELLO SEGA, Department of Computational Biological Chemistry, University of Vienna — A variety of biological and technological problems where long chain molecules are constrained in spaces small compared to the molecule size (like membrane nanopores or nanofluidic slits) motivated recently a growing effort to understand the dynamics and structural scaling properties of polymers confined by solid walls. Our focus is, instead, on polymers confined in different geometries by soft interfaces, mimicking, e.g., DNA packaging inside cell nuclei or, mutatis mutandis, viral capsids. Soft-confinement is achieved by a proper choice of the solvation energies such that the polymer is trapped in one of the two phases of a binary mixture of immiscible liquids. We perform Molecular Dynamics simulations of polymers coupled with a fluctuating lattice Boltzmann method for the embedding matrix. Slab and droplet configurations are considered. In the former case we address the transition among various regimes of size scaling at changing the slab width. Under shear, the droplet is distorted from its equilibrium spherical shape and we explore how the transition from an isotropic geometry to a quasi-tube-like one affects polymer size scaling and knotting degree. Finally, we show how the feedback on the solvent induces viscoelastic rheology that can be related to polymer entanglement.

Andrea Scagliarini
Department of Physics, University of Rome "Tor Vergata"

Date submitted: 11 Nov 2014 Electronic form version 1.4