ADSORPTION AND TRIBOLOGY OF MOLECULES ON AND BETWEEN SURFACES

Recent coarse-grained simulation studies of various aspects of molecular adsorption and tribology will be reported. The physisorption of linear and star polymers on smooth surfaces will be discussed. Emphasis will be placed on the comparison between simulation results and the predictions of scaling theories for the structures of the adsorbed layers [1,2]. The kinetic friction arising from an oil-like fluid layer confined between sheared parallel surfaces will be considered next. Of particular note is an observed logarithmic dependence of the kinetic-friction coefficient on shear rate. The effects of small concentrations of amphiphilic additives on the kinetic friction will be described and correlated with the steady-state distribution of additive molecules throughout the fluid layer [3]. Finally, some outstanding problems and ongoing work in this broad area will be outlined.

[1] "Adsorption and self-assembly of linear polymers on surfaces: A computer simulation study", A. Chremos, E. Glynos, V. Koutsos, and P. J. Camp, Soft Matter 5, 637-645 (2009).

[2] "Adsorption of star polymers: computer simulations", A. Chremos, P. J. Camp, E. Glynos, and V. Koutsos, Soft Matter 6, 1483-1493 (2010).

[3] "Molecular simulations of kinetic-friction modification in nanoscale fluid layers", M. R. Farrow, A. Chremos, P. J. Camp, S. G. Harris, and R. F. Watts (submitted).