Speaker: Emanuele Locatelli (Università di Padova, Italy)

Title: Adsorption properties of polymeric brushes in and out of equilibrium

Abstract: We consider polymer brushes able to adsorb colloidal-like solutes and we study, using computer simulations and scaling theory, their conformational and adsorption properties in and out of equilibrium. In equilibrium, Langevin Dynamics simulations show, with increasing the amount of solute, the collapse of the brush followed by a successive re-swelling. We rationalize this phenomenology through a scaling theory, following Alexander and de Gennes, where adsorption is seen as a progressive worsening of the solvent conditions[1]. Going towards practical applications, we study adsorption out-of-equilibrium introducing fluid flow and hydrodynamic interactions. We find that increasing colloid flux, either by an increase in
applied pressure or colloid density, unexpectedly promotes adsorption[2].

[1] C. F., Vorsmann, S. Del Galdo, B. Capone, and E. Locatelli, Colloidal adsorption in planar polymeric brushes, Nanoscale Advances, 6 (2024) 816-825.
[2] C. F., Vorsmann, E. Orlandini, and E. Locatelli, Colloidal adsorption in functionalized nano-channels, In preparation (2025)