MODELING ADSORPTION ON BIOMIMETIC SURFACES FOR THE DEVELOPMENT OF ENVIRONMENTALLY FRIENDLY POLYMER COATINGS

Arturo Moncho-Jorda*
Biocolloid and Fluid Physics Group, University of Granada, Granada, Spain and
Institute Carlos I for Theoretical and Computational Physics, University of Granada, Granada, Spain

Jose Lopez-Molina and Irene Adroher-Benitez†
Biocolloid and Fluid Physics Group, University of Granada, Granada, Spain

Nicolas A. Garcia
Instituto de Fisica del Sur, CONICET, Bahia Blanca, Argentina and
Departamento de Fisica, Universidad Nacional del Sur, Bahia Blanca, Argentina

Jean-Louis Barrat
Laboratoire Interdisciplinaire de Physique, Universite Grenoble Alpes-CNRS, Grenoble, France and
Institut Laue-Langevin, Grenoble, France

Gustavo S. Luengo and Fabien Leonforte
L'Oréal Research and Innovation, Aulnay-Sous Bois, France

Adsorption of polymers on heterogeneous, biologically inspired surfaces is a multiscale problem that links molecular design with macroscopic function. We developed a computational framework based on coarse-grained molecular dynamics to study how polymer architecture, chain length, and concentration controlled the formation and stability of polymer coatings on complex substrates. The model substrate was a digital replica of the fatty F-layer that protects human hair, obtained from high-resolution microscopy data [1]. Two representative polymers were examined: a linear flexible chain that illustrates emerging bio-based candidates for cosmetic applications, and a stiff comb-like cationic polyelectrolyte typical of current high-performance films.

Equilibrium simulations showed that increasing bulk concentration always enhanced adsorption, yet architectural differences strongly affected film morphology. The branched polyelectrolyte built thicker and more uniform layers, whereas the linear polymer reproduced the surface heterogeneity of the substrate. A slab-wise density analysis quantified this partial coverage and highlighted regions where the film was locally depleted or enriched. To probe mechanical resistance, we subjected the adsorbed layers to linear shear flow. Tracking the fraction of adsorbed chains in time revealed that even weak shear induced partial desorption, while strong shear accelerated this process. For both polymer types, longer chains conferred greater resistance, but the comb-like architecture remained more stable overall [2]. We then extended the study to interfacial friction. Symmetrical substrates, each coated with identical polymer films taken from the adsorption runs, were compressed to selected separations and then slid past one another. By varying polymer architecture, chain length, inter-layer distance, and sliding velocity, we aimed to map the kinetic friction coefficient and relate it to film morphology.

The methodology introduced here provides transferable tools for exploring adsorption-desorption and friction phenomena in polymer systems, offering quantitative guidelines for designing sustainable coatings that operate reliably under realistic conditions.

---

[1] T.I. Morozova et al., *ACS Appl. Mater. Interfaces* **13**, 30086 (2021).
[2] I. Adroher-Benitez et al., *Macromolecules* **56**, 10285 (2023).

* moncho@ugr.es
† iadroher@ugr.es