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All-Atom Modeling and Simulation of Bio-Polymer Interface: Dual Role of Antifouling Polymer Brushes

Antifouling polymers are highly valuable in a variety of applications, including antiviral coatings, targeted drug delivery, and marine coatings, where preventing unwanted protein adsorption is critical. Although extensive experimental studies have characterized polymer-protein interactions, computational studies remain limited due to the difficulty and complexity of integrating and investigating those two different components into a single system. This study presents molecular modeling and simulation of polyelectrolyte and polyzwitterionic brushes—poly(dimethylaminoethyl methacrylate) (PDMAEMA), poly(2-(N-oxide-N,N-dimethylamino)ethyl methacrylate) (PNOMA), and poly(2-(N-3-sulfopropyl-N,N-dimethylammonium)ethyl methacrylate) (PSBMA)—grafted onto α-quartz substrates. The brush models were developed to closely replicate experimentally synthesized brush samples and to provide detailed insights into structural and dynamical changes at the molecular level during protein adsorption. Using steered molecular dynamics simulations, we show that the PSBMA brush, due to its high local density, exhibits the greatest resistance to protein insertion. C⍰ root-mean-square deviation and interaction patterns analyses further reveal that PSBMA also induces the most significant destabilization of lysozyme, while PDMAEMA brush enhances protein stability through ion-mediated interactions. The PNOMA brush, while requiring the lowest force for protein adsorption, induces greater protein destabilization than the PDMAEMA brush primarily due to electrostatic repulsion caused by a shorter carbon spacer length. To the best of our knowledge, this study represents the first comprehensive and realistic model system—comprising nanomaterials, polymers, and proteins, specifically antifouling polyzwitterions and polyelectrolytes grafted onto ⍰-quartz substrates via linkers. These findings highlight the dual role of antifouling polymer brushes: resisting protein adsorption and modulating protein structural dynamics, offering valuable insights for the rational design of next-generation antifouling materials.

Topical Area

Soft matter: polymers, and complex fluids

Author: KIM, Seonghan (CNMS)

Co-authors: YANG, Zhefei (CNMS); SOLSONA, Ruben Millan (CNMS); WANG, Hanyu (CNMS); JAKOWSKI, Jacek (CNMS); GANESH, Panchapakesan (CNMS); RETTERER, Scott (CNMS); CARRILLO, Jan-Michael (CNMS)

Presenter: KIM, Seonghan (CNMS)