Simulations at the interface: protein association in lipid membranes, polymer adsorption on surfaces and reaction-diffusion in polymer films.

Rapid advances in fields ranging from biology to nano-structured materials have revealed a greater need for fundamental understanding at molecular length scales. Computer simulations are increasingly applied to study interfacial phenomena with new efficient techniques aiming to overcome the challenges associated with such heterogeneous systems. In this talk we focus on efficient algorithms and multiscale models to study diverse systems such as proteins and their association in membrane environments, interactions of macromolecules with surfaces and reaction-diffusion phenomena in polymer thin films. Particular emphasis will be given to techniques developed to advance our knowledge on the role of chemical constitution and architecture to the observed behavior. Specific results presented will demonstrate the unique contribution of modeling when coupled with experimental investigation, in establishing the connection between molecular detail and macroscopic material properties.