Physical Chemistry Seminar

Polymer Surfaces for Fouling-Resistant Coatings and Nanofiltration Membranes

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Understanding interfacial phenomena of polymers has many applications, including fouling-resistant coatings, biomedical implants, drug delivery, and nanofiltration for water treatment and gas separation. To achieve structure–function design, we employ multiscale simulations ranging from quantum to atomistic to mesoscopic scales, in combination with experiments at the intersection of chemistry, physics, and biology. Two projects will be presented to illustrate how we address different aspects of interfacial phenomena and facilitate experimental design of polymer surfaces: (1) antibiofouling zwitterionic polymers and (2) reverse osmosis (RO) polyamide membranes.

Zwitterionic polymers, which contain equal numbers of positively and negatively charged groups, have emerged as a highly effective class of environmentally friendly and biocompatible coating materials for resisting marine biofouling on vessel surfaces and protein corona formation in drug delivery. Our multiscale simulations revealed that interfacial hydration, the charge distribution of zwitterions, and surface structure are crucial to the antibiofouling performance of zwitterionic polymer surfaces.

Polyamide RO membranes are among the most successfully commercialized technologies for desalination and water purification. Our simulations revealed the interfacial cross-linking mechanism and the relationship between membrane microstructure and performance, which are important to experimental synthesis. Our study showed that the solution interface concentrates monomers during the initial stage of rapid cross-linking and disperses them during the subsequent slower stage to promote the formation of cross-linked membrane structures. The interactions among aromatic benzene rings govern the membrane's nanoporous microstructure and control water permeation and salt separation.

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PURDUE UNIVERSITY

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Dr. Tao Wei is an associate professor in the Biomedical Engineering Department and Chemical Engineering Department at the University of South Carolina. Dr. Wei got his PhD degree from University of Southern California. Dr. Wei's research focuses on functional materials and biotechnologies using the combination of multiscale simulations, experiments and machine learning. Dr. Wei is a recipient of NSF CAREER award in 2020. His projects on abiotic-biotic interfacial Redox, antibiofouling and fouling release materials, polymer membrane, bionanotechnologies, biosensor development, and hydrogen conversion have been funded by NSF, ONR, NASA and DOE.