"Molecular Structures of Polymer and Biological Molecules at Buried Interfaces"

Solid/solid and solid/liquid interfaces are difficult to study in situ because they are buried. We have developed a systematic way to probe such interfaces in situ in real time at the molecular level using a nonlinear optical spectroscopy, sum frequency generation (SFG) vibrational spectroscopy. This talk will focus on our recent progress in applying SFG to study molecular orientations of semiconducting polymers at buried solid/solid interfaces, surface immobilized peptides and enzymes in different chemical environments, and molecular interactions between 2D materials (e.g., graphene, MoS2, WS2) and biological molecules. Our SFG studies are supplemented by attenuated total reflectance (ATR)-FTIR and circular dichroism (CD) spectroscopy as well as all-atom and coarse-grain molecular dynamics simulations. It was found that interfacial orientations of semiconducting polymers are influenced by polymer side chains and substrate surface hydrophobicity, and such interfacial orientations are well correlated to polymer solar cell conversion efficiency. Biological molecules interact with different 2D materials very differently. On graphene, pi-pi interactions play an important role. On MoS2, hydrophobic interaction is the determining factor. Using SFG, we also elucidated the effects of protein surface immobilization sites, chemical environments, and substrate surface properties on the structures and properties of surface immobilized enzymes.