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Polymers at Surfaces and Interfaces[1]

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Interfaces between solids, liquids, and gases play an important role in a wide range of practical applications and have been a subject of scientific interest since Poisson showed in 1831 that the order parameter of liquids near interfaces must deviate considerably from its bulk value. In particular, polymers at surfaces and interfaces have been a subject of extensive theoretical, experimental and computational studies for a long time due to their use in many diverse applications ranging from antifouling coatings to flexible electronic devices. Understanding the structure and thermodynamic properties of polymers at surfaces and interfaces is thus an area of fundamental and current technological interest. Although encouraging experimental progress has been made over the years in understanding the molecular structure of polymers in contact with various environments, selectively probing their structure and dynamics at surfaces and interfaces has been extremely difficult. Computer simulations, especially molecular dynamics (MD) simulations, have proven over the years to be an invaluable tool in providing molecular details at interfaces that are usually lacking in the experimental data. In this talk, I'll give an overview of some previous simulation efforts to understand the structure and dynamics of polymers at surfaces and buried interfaces. I will conclude by presenting our current and ongoing work on combining ab initio calculations and MD simulations with Sum Frequency Generation (SFG) Spectroscopy to study polymer surfaces. This approach demonstrates the future role of MD in surface science.

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