Multiscale Modeling of Polymers at Interfaces

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Abstract:
Many industrially important phenomena, such as wetting, adhesion, friction, and mechanical contact, all depend significantly on the molecular structure and properties of the materials under investigation. Polymers remain among the most difficult classes of materials to successfully model, because of their intrinsically multiscale nature, and the importance of the monomer structure on their macroscale properties. Studies of physical phenomena occurring at interfaces is similarly challenging, because many of the assumptions used to parameterize the force fields used in molecular simulation are no longer applicable. We will discuss methods developed in our group to address the challenges of simulating the behavior of polymers at interfaces, both at the atomistic and the continuum scales. For instance, modeling the surfactant-enhanced spreading of water droplets required the development of efficient solvers for long-ranged dispersion forces near interfaces, which have traditionally been ignored in molecular simulations, as well as the adoption of tools from the image processing community to analyze the shape and structure of the droplets as they spread. Similarly, construction of continuum models of nanoindentation in self-assembled monolayers requires successful parameterization of the required material models; we show how these can be efficiently extracted from carefully constructed molecular dynamics simulations.

Bio:
Prof. Ahmed E. Ismail is currently a Junior Professor in the Faculty of Mechanical Engineering at RWTH Aachen University in Aachen, Germany. He earned his bachelor's degree in Chemical Engineering from Yale University in 1998. As a PhD student in Chemical Engineering at MIT in the Rutledge and Stephanopoulos groups, he was the recipient of fellowships from the DOD NDSEG and the DOE Computational Science Graduate Fellowship programs. He received his PhD in 2005 before beginning a postdoctoral position at Sandia National Laboratories working with Gary Grest and Mark Stevens. From 2006 to 2010, he was a Senior Member of Technical Staff at Sandia, working as an environmental engineer for the Waste Isolation Pilot Plant program. The current research interests of Prof. Ismail's group include modeling of biomass dissolution, polymers, and interfacial phenomena, as well as algorithm development to support these application areas.