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SEMINAR SERIES

Wednesday, June 5, 2024
Seminar Presentation: 11:00am – 12:00pm
SME Room 248

"How Do Polymers Wiggle? Understanding the Dynamics of Grafted Polymers"

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Abstract: Grafted polymers are vital components in various soft materials, utilized for applications ranging from enhancing the mechanical properties of nanocomposites to optimizing immune responses for new macromolecular therapeutics. In this talk, I will detail our recent computational studies on the relaxation dynamics of grafted polymers in two distinct systems: (1) surface-grafted polymers and (2) linear polymer backbones densely grafted with short side chains, also known as molecular bottlebrushes or graft polymers. When grafted onto surfaces, polymers can adopt a wide array of conformations, influenced by factors such as grafting density and the curvature of the underlying surface. In contrast, molecular bottlebrushes retain many of the characteristics of free linear polymers, yet they also display unique behaviors due to their grafted side chains. These side chains cause the backbones of the bottlebrushes to extend, leading to behaviors that include slower relaxation dynamics and very high entanglement molecular weights. The specific grafting conditions in both systems significantly alter the fundamental modes that govern the motion and relaxation of the polymers. This complexity requires the use of advanced, data-driven methods like the Proper Orthogonal Decomposition (POD) for correct analysis of the simulation results. The results of our simulations are compared to prior neutron scattering studies conducted by our group as well as others in the polymer community.

Biosketch: Michael J. A. Hore is the Warren E. Rupp Associate Professor in the Department of Macromolecular Science and Engineering at Case Western Reserve University. He completed his undergraduate studies in Physics/Mathematics and earned a Master's degree in Physics at The University of Memphis. He received his Ph.D. in Materials Science & Engineering from the University of Pennsylvania in 2012 under the guidance of Professor Russ Composto. Following his doctoral studies, he accepted a National Research Council (NRC) Postdoctoral Associateship at the NIST Center for Neutron Research (NCNR) in Gaithersburg, MD, where he focused on neutron scattering measurements of macromolecular systems.

Professor Hore has been honored with several teaching awards and recognitions of his research, including an NSF CAREER Award, the DPOLY/UKPPG Lecture Exchange Award from the American Physical Society, and designation as a 2018 PMSE Young Investigator by the PMSE Division of the American Chemical Society. His research group blends theory, computer simulations, and experimental studies to investigate topics such as grafted polymers, molecular bottlebrushes, thermoresponsive materials, and nanoparticle transport.