ME Seminar

Computational Design of Polymer Composites: Molecular Simulations for High-Performance Applications

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ABSTRACT

The demand for next-generation aerospace materials is driving the development of lightweight, ultra-strong, and multifunctional composites. With long-duration missions, including Mars expeditions, on the horizon, materials must combine exceptional mechanical performance with low weight and high reliability. Computational modeling provides a powerful tool to accelerate this development by revealing molecular mechanisms underlying macroscopic behavior.

This research integrates multi-scale modeling within an Integrated Computational Materials Engineering (ICME) framework to predict property evolution during composite processing and use. Molecular dynamics (MD) simulations with a reactive force field (IFF-R) were employed to model the curing of an epoxy system. Property predictions were generated as a function of crosslink density, revealing non-linear, property-specific trends. These results inform higher-scale process-structure-property models. Further studies investigated interfacial behavior in composites reinforced with flattened carbon nanotubes (flCNTs). MD simulations evaluated interaction energy, sliding resistance, and transverse binding strength with three polymers: epoxy, bismaleimide (BMI), and benzoxazine. BMI showed the strongest interfacial adhesion and transverse strength, positioning it as a promising matrix for flCNT-based composites. Additional work focused on epoxy nanocomposites reinforced with graphene quantum dots (GQDs). Functionalization with hydroxyl groups significantly enhanced stiffness and yield strength by 18.4% and 56.1%, respectively, due to improved molecular packing and reduced free volume.

Together, these studies demonstrate a cohesive computational approach for designing high-performance composites, with broad applications in aerospace, energy, and other advanced engineering systems.

ABOUT THE SPEAKER

Prathamesh Deshpande is a computational materials scientist with over nine years of research experience in computational mechanics and materials science. He holds a Ph.D. in Mechanical Engineering–Engineering Mechanics from Michigan Technological University, where his doctoral research focused on molecular modeling of high-performance polymer composites. He also holds a master's degree from Michigan Technological University and a bachelor's degree in Mechanical Engineering from the University of Pune, India. His core expertise lies in atomistic and quantum modeling (molecular dynamics, density functional theory), continuum-level modeling (finite element analysis), and multiscale simulation frameworks. He has also developed application-driven codebases and conducted extensive data analysis to support predictive materials design. Most recently, he served as a Postdoctoral Research Associate at the San Jose State University Research Foundation, where he contributed to several interdisciplinary projects. Prathamesh was a contributing member of the NASA STRI: Institute for Ultra-Strong Composites by Computational Design (US-COMP), a $15 million research initiative focused on developing next-generation aerospace materials. His research has been published in multiple peer-reviewed journals and presented at leading international conferences. In addition to his technical contributions, he has demonstrated leadership and advocacy as the former Vice President of the Graduate Student Government at Michigan Technological University, where he promoted academic and community engagement among graduate students.

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