ME Seminar

Molecular Modelling of Materials for Aerospace Applications

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ABSTRACT

There is an increasing demand for lightweight structural materials in the aerospace industry to facilitate more efficient and cost-effective space travel. Polymer matrix composites (PMCs) reinforced with carbon nanotubes (CNTs) have demonstrated significant improvements in mechanical performance. Among them, flattened carbon nanotubes (flCNTs)—key components of CNT yarns and sheets—have emerged as promising candidates for ultra-strong composites.

However, during CNT yarn synthesis, traces of amorphous carbon (AC) are often present, potentially compromising composite strength. Understanding the influence of these impurities is essential for optimizing composite properties. As experimental investigations can be costly and time-intensive, this research employs molecular dynamics (MD) simulations to evaluate interfacial interactions between flCNTs and AC, offering insights into atomic-scale behavior.

These computational tools not only yield accurate predictions but also significantly reduce development time and cost, thus accelerating the design of next-generation aerospace composites.

ABOUT THE SPEAKER

Dr. Prashik Sunil Gaikwad is currently a Research Fellow in the Chemistry Department at the University of Warwick, UK, where he works on solid-state battery materials using density functional theory (DFT) and machine learning. He completed his Ph.D. in Mechanical Engineering at Michigan Technological University (2023), focusing on molecular dynamics simulations of nanocomposite materials.

He holds an M.S. in Mechanical Engineering from the University of Texas at Arlington and a B.E. in Mechanical Engineering from Savitribai Phule Pune University. He has previously held research positions at Microvast Inc., Idaho National Laboratory, and Michigan Tech, where he contributed to modeling efforts in battery materials, solid oxide electrolysis cells, and polymer composites.

Dr. Gaikwad has authored over ten peer-reviewed publications, delivered multiple conference presentations, and received the Dean's Award for Outstanding Graduate Scholarship (2023) and the NASA Research Excellence Award (2023). His work integrates atomistic modeling with engineering applications, with a strong focus on energy and aerospace materials.

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