Polymer Interphases: A Case for Multiscale Modelling

Florian Müller-Plathe
Theoretical Physical Chemistry
Technische Universität - Darmstadt, Germany

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Seminar host: Ganesh Balasubramanian
*Please note this seminar takes place on Friday, not Tuesday*

Abstract
Polymers in contact with solid surfaces, such as encountered in adhesives, coatings or nanocomposites develop a peculiar region close to the solid, where their properties are not quite bulk-like. Little is known about the molecular structure and dynamics of this so-called interphase and about the local polymer properties. On the one hand, the features of the interphase seem to depend on subtleties of the molecular interactions; on the other hand, the interphase can be wide. For this reason, simulations of a single resolution are not sufficient, and we have used anything from atomistic molecular dynamics to finite elements. This talk reports theoretical findings about the nature of the interphase, as mapped out by monitoring different quantities and their profiles near the solid. Where possible, they have been matched against experiments.

Florian Müller-Plathe is Professor of Theoretical Physical Chemistry at Technische Universität Darmstadt, Germany. He has worked on the molecular simulation of fluids, polymers and materials for more than 25 years, with major method development efforts in multiscale modelling and coarse-graining, transport properties, as well as the molecular characterization of interfaces and interphases. After studying chemistry at Ludwig-Maximilian University Munich (D) and obtaining a PhD from the Technical University of Munich (D), he worked in various capacities at Daresbury Laboratory (UK), ETH Zürich (CH), Max-Planck Institute for Polymer Research Mainz (D) and Jacobs-University Bremen (D). He is a regular member of the Academy of Sciences and Literature Mainz (D).

This seminar counts towards the ME 600 seminar requirement for Mechanical Engineering graduate students.

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