הטכניון - מכון טכנולוגי לישראל

TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY

הפקולטה להנדסה כימית
ע"ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar
Lecture Hall 6, Wolfson Department of Chemical Engineering,
Wednesday December 11, 2019 at 13:30

Viscoelastic Properties Prediction of Fluoropolymers through Multiscale Modeling

Erez Tamir

Advisors: Prof. Yachin Cohen, Dr. Arieh Sidess, Prof. Simcha Srebnik

The time-dependent mechanical behavior of polymers subjected to continuous stress is an engineering issue of high importance and great relevance to industrial applications. The mechanical behavior is governed by molecular characteristics of the polymer (i.e., atomic structure and molecular weight). Therefore, it is extremely important to develop prediction capabilities of the time-dependent response of polymers, by linking the molecular structure to macroscopic properties.

The aim of this research is to develop a multiscale bottom-up modeling procedure for fluoropolymers up to mesoscopic length and timescales in order to predict viscoelastic properties such as stress relaxation. Molecular dynamics simulations will be performed first in order to calculate thermodynamic and dynamic properties of atomistic models. Several atomistic potentials (force-fields) will be compared, and the calculated properties will be compared to experiments. Next, Coarse-graining will be carried out in order to reach mesoscopic properties.

Refreshments will be served at 13:15