



**Wolfson Department of Chemical Engineering Seminar**  
**Lecture Hall 6, Wolfson Department of Chemical Engineering,**  
**Wednesday May 10<sup>th</sup> at 1:30pm**

**Irena Levin**

**PhD candidate (advisor: Prof. Yachin Cohen)**  
**Chemical Engineering, Technion**

**Polymer adsorption on the surface of carbon nanotubes**

Carbon nanotubes (CNTs) possess unique properties leading to many potential applications, such as composite materials. However, due to their strong tendency to agglomerate, the quality of their dispersion in the processing liquid is crucial for obtaining the desired distribution and functionality in the final composite. Physical adsorption of polymers on CNTs, through specific interfacial interactions, hinders their aggregation and improves the compatibility of CNTs with the polymer matrix thus strengthening their interface. Stable homogeneous dispersions of multi-walled carbon nanotubes (MWNTs) in N,N-dimethyl formamide (DMF) were achieved by physical modification of the MWNT surface using several block copolymers, with various molecular weights and chemical structures. The dispersions were imaged by cryogenic transmission electron microscopy (cryo-TEM) for qualitative evaluation of the CNT distribution. Structural information on the MWNT/copolymer hybrid was achieved by detailed small angle neutron scattering (SANS) measurements using contrast variation, with particular emphasis on the conformation and adsorption density of the copolymers on the MWNT surface. The various contrasts were achieved by suitable mixing of natural and deuterated solvent molecules, thereby highlighting different parts of the structure.

**Erez Tamir**

**PhD candidate (advisor: Prof. Simcha Srebnik)**  
**Chemical Engineering, Technion**

**Viscoelastic properties prediction of fluoropolymers through multiscale modeling**

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 analyze amorphous polymers of various structures and molecular weights distributions. Molecular dynamics simulations will be performed first in order to calculate thermodynamic and dynamic properties of atomistic models. Next, Coarse-graining will be carried out on several levels in order to reach mesoscopic properties.

Refreshments will be served at 13:15