Network for Computational Nanotechnology
& c-PRIMED Seminar Series

PURDUE UNIVERSITY Discovery Park

Dr. Nasim Anousheh

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Monday, January 8th at 11am
Birck Nanotechnology Center, Room 1001

Atomistic simulation of fluoropolymers: the influence of regiodefects on the characterization of polyvinylidene fluoride

Alternating two groups, CH2 and CF2, of very different polarities along the backbone chain of polyvinylidene fluoride (PVDF) leads to very interesting properties, such as ferroelectricity. However, these properties are affected by the presence of regioisomerism defects (monomer inversion) that appear during the synthesis. During the polymerization, in addition to the Head-to-Tail (HT) sequences, CH2CF2CH2CF2, the reversed monomer units lead to formation of Tail-to-Tail (TT), CF2CH2CH2CF2, and Head-to-Head (HH), CH2CF2CF2CH2, links. The percentage of these defects in most commercial PVDF samples is between 3 and 7 %. This percentage undoubtedly brings changes in macroscopic properties. The aim of this presentation is to reveal the impact of these defects on the glass transition temperature (Tg), local dynamics and melting temperature (Tm) of PVDF. To study these phenomena we use Molecular Dynamics simulation. To highlight their role in modifying polymer chain relaxation, the activation energy (Ea) related with conformational transitions is computed. From the relation between the conformational transition and the glass transition, the Tg of the alternate copolymer ethylene tetrafluoroethylene (E-TFE), an isomeric polymer of PVDF, can be deduced. Tg of this copolymer (E-TFE) is still source of discussion in the literature.

Dr. Nasim Anousheh is currently a Visiting Scholar at Professor Vikram Jadhao's Research Group, at Indiana University (USA). She received her PhD in Physical Chemistry from the University of Sherbrooke (Canada) at Laboratory of Physical Chemistry of Matter (LPCM), under supervision of Professor Armand Soldera. Her PhD thesis entitled "Atomistic Simulation of Fluoropolymers: Impact of Regio-defects on Characterization of Polyvinylidene Fluoride" addresses the molecular simulation of polymers. The objective of this thesis was to understand the link between molecular and macroscopic systems of polymers by combining simulation, experiments and theory. This makes it possible to predict and design new materials with improved properties. During her PhD, she had the honor of being a co-author in the book entitled "Handbook of Fluoropolymer Science and Technology". She is also the author of several publications in renowned international journals including Polymer and Polymer Science.