



学术报告



Nano tools for macro problems: *multiscale molecular modeling of nanostructured polymer systems*

嘉宾： Prof. Maurizio Fermeglia

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嘉宾简介：

Maurizio Fermeglia is full professor at the Department of Engineering and Architecture of the University of Trieste, where he holds the course in Chemical and Biochemical Reaction Engineering and Process and Product design. From 2006 to 2012 he was the head of the Department of Industrial Engineering & Information Technology, from 2010 to 2012 he served as president of the Research board of the University of Trieste. He was the director of the Ph.D. School of Nanotechnology at the University of Trieste from 2007 to 2013. From 2013 to 2019, he was the Rector of the University of Trieste. His research interests are focused on multiscale modeling for materials design and life science, applied thermodynamics, process simulation, molecular modeling for nanotechnology and nanomedicine.

Maurizio Fermeglia is member of the EFCE working party on thermodynamics and transport properties, IUPAC fellows, member of the AIChE, member of Italian associations GRICU and AIDIC. He received the Italy meets Asia Science Award in 2015. He was scientific consultant of ICS - UNIDO within the Subprogram 'Process Simulation and sustainable development' from 1999 to 2011 and of UNEP for the implementation of PRTR in different countries from 2005 to 2013.

报告内容：

One of the major goals of computational material science is the rapid and accurate prediction of properties of new materials. Despite the tremendous advances made in the modeling of structural, thermal, mechanical and transport properties of materials at the macroscopic level, there remains a tremendous uncertainty about how to predict many critical properties related to performance, which strongly depends on nanostructure. It is then essential to analyze the structure at molecular level, with all the chemical biological and physical implication. Currently, atomistic level simulations such as molecular dynamics (MD) or Monte Carlo (MC) techniques allows to predict the structure and properties for systems of considerably large number of atoms and time scales of the order of microseconds. Although this can lead to many relevant results in material and system design, many critical issues still require time and length scales far too large for practical MD/MC simulations. This requires developing techniques useful to design engineers, by incorporating the methods and results of the lower scales (e.g., MD) to mesoscale simulations. In this work, we present applications of multiscale modeling procedures for predicting macroscopic properties strongly depending of interactions at nanoscale scale. Several different polymer systems of interest in the area of materials sciences and life sciences will be considered, including (i) functionalized nanoparticles in un structured polymer matrices (effect of chain length and grafting density on the grafted nanoparticle, computer simulation of polyurethane foams, design of nanostructured membranes), (ii) functionalized nanoparticles in nanostructured polymer matrices (localization of gold nanoparticles in di-block copolymers and selective placement of magnetic nanoparticles in diblock copolymer films), and (iii) self-assembly organization for biomedical applications (multivalent self-assembly building blocks in nanoparticles).