NOMATEN HYBRID-SEMINAR

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In-person: NOMATEN seminar room

Tuesday, MARCH 7th 2023 13:00 CET

Insight into molecular dynamics behavior of glass-forming liquids from experiment and MD simulations.

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Abstract: At the beginning we will have a brief look at the liquid-glass transition phenomenon. However, most attention will be focused on the behavior of molecular dynamics during the vitrification process, caused by cooling and compression. Molecular dynamic behavior will be analyzed and discussed mainly in term of the density scaling idea, which was proposed to jointly describe the dependence of molecular dynamics of glass-forming liquids on thermal and packing effects. According to this idea, both isobaric and isothermal structural relaxation times or viscosity can be expressed as a single universal curve if they are plotted against new variable TV^{γ}, where T and V denote temperature and specific volume, respectively, and γ is the scaling exponent. The core of my presentation will refer to the relationship between the scaling exponent, the steepness of the repulsive part of the intermolecular potential, and the role of molecular structure and interaction anisotropy. In the last part of my presentation, I will also show how density scaling can be applied to analyze entropy data.

Bio: Professor of Physics at the Institute of Physic, Department of Science and Technology of the University of Silesia in Katowice, Director of the Silesian Center for Education and Interdisciplinary Research.
For two years he worked at the Polymer Research Institute, in the team of prof. E. W. Fischer at the Max Planck Institute in Mainz. He also worked as a Visiting Professor at the Naval Research Laboratory in Washington, the University of Akron, the Hebrew University, the University of Pisa and the University of Tennessee. Since January 2010 he has been serving as Associate Editor in AIP Advances which is an open-access peer-reviewed scientific journal published by the American Institute of Physics. Moreover, since 2020 he has been acting as a member of the Editorial Advisory Board in Molecular Pharmaceutics.
A world-renowned specialist in the field of molecular dynamics studies of glass-forming liquids and polymer melts. His key achievements in generation of knowledge in this field are closely connected with developed by him high pressure apparatus for dielectric spectroscopy measurements. His major accomplishment in the field of glass transition using high pressure was establishing relationship between the importance of thermal energy and free-volume contributions to the molecular dynamics near the glass transition and strength and type of intermolecular interactions. He also applied his experimental technique to the study ionic liquids and polymerized ionic liquids, with the objective of making contribution to deeper understanding of the charge transport in these important systems.
Generated knowledge from the studies of these two mentioned topics was thoroughly described in two books:

1. “Molecular Dynamics of Glass-Forming Systems – Effect of Pressure”, Springer-Verlag 2011
2. “Dielectric properties of Ionic Liquids”, Springer-Verlag 2016

In last decade, his scientific interests have focused on researching the molecular mechanisms responsible for the physical stability of amorphous drugs. His achievements in this field have gained international recognition.

His scientific works are published in the most prestigious scientific journals such as: Macromolecules, Physical Review Letters, JACS, Journal of Physical Chemistry Letters, Molecular Pharmaceutics, Physical Chemistry Chemical Physics, Nature Communication, etc.. Professor Paluch is the author of over 500 scientific articles. His publications were cited over 17000 times.