Non-affine lattice dynamics approach to measure viscosity in polymeric systems

Ankit Singh*[1], Vinay Vaibhav[1], and Alessio Zaccone†[1]

[1]Department of Physics "A. Pontremoli", University of Milan, via Celoria 16, 20133 Milan, Italy – Italy

Abstract

Viscosity, a fundamental rheological property of liquids, quantifies the resistance to relative motion between molecular layers and plays a critical role in understanding material behavior. Conventional methods, such as the Green-Kubo (GK) approach, rely on time integration of correlation functions, which becomes computationally intensive near the glass transition due to slow correlation decay. A recently proposed method based on non-affine lattice dynamics (NALD) (1) and instantaneous normal mode analysis offers a promising alternative for estimating viscosity. In this study, we apply the NALD approach to compute the viscosity of the Kremer-Grest polymer system over a range of temperatures and compare these results with those from the GK method and non-equilibrium molecular dynamics simulations. Our findings reveal that all vibration modes, including the instantaneous normal modes, contribute to viscosity. Furthermore, we investigate the role of microscopic friction in determining viscosity. This work presents an efficient framework for calculating viscosity across diverse systems and opens the avenue to understanding the role of different vibrational modes linked with structure, facilitating the design of materials with tunable rheological properties.
References:

(1) A. Zaccone, Phys. Rev. E 108, 044101 (2023).

*Speaker

†Corresponding author: alessio.zaccone@unimi.it