Stress fluctuations, shear modulus and phase transitions

Hong XU

Laboratory LCP-A2MC, 1 Bd Arago, Univ. Lorraine, 57070 Metz, France

E–mail: hong.xu@univ-lorraine.fr

In this presentation we shall review some recent progress and applications of the stress fluctuation formalism. In particular, we show how the shear stress relaxation modulus can be computed accurately in equilibrium molecular dynamics simulations [1]. Then we shall investigate the temperature dependence of the shear modulus, especially through the glass transition [2], in order to compare to predictions of the mode coupling theory, and experimental estimates. Last, we present recent results on linear viscoelasticity of a model glass former [3], in liquid and solid states, and discuss our results in terms of simple rheological models.

References

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(2) D. Li, H. Xu and J.P. Wittmer, J. Phys. Cond. Matt. 28 (2016)
(3) D. Li, O. Greffier and H. Xu, Mol. Phys. (2019)