

INSTITUTE COLLOQUIUM

TITLE : *The Elusive Connection Between Structure and Dynamics in the Supercooled Liquids*

*10th September,
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4.00 PM*

Speaker :: *Dr. Sarika Maitra Bhattacharyya,
Sr. Principal Scientist, Professor ACSIR,
CSIR-National Chemical Laboratory, Pune*



ABSTRACT :: *In theories of liquids the structure provides information of the thermodynamic and dynamic quantities. However, in supercooled liquid although the dynamics changes over orders of magnitude, the change in the structure is small, and this observation raises the question about the role of structure in the dynamics. Studies showing that two systems with very similar structures have orders of magnitude difference in dynamics at low temperatures further strengthen the argument that pair structure does not play any role in the slowing down of the dynamics. The common wisdom in supercooled liquid community is that many body correlation drives the slowing down of the dynamics. Based on our work, I will present a completely new and counter intuitive understanding of the role of pair and higher order correlations in the dynamics. We find that slow dynamics in supercooled liquid is driven by the pair correlation and many body correlation helps the system to explore larger phase space and speed up the dynamics [1]. Motivated by our work in a recent study, the role structure was revisited [3]. A softness parameter was described which is a weighted integral of the structure where the weight is obtained from the dynamics using machine learning (ML) techniques [3, 4]. The study shows that for systems having similar structure this softness varies and the dynamics for two systems when plotted against the softness, shows a master plot. Despite the success of the ML study in connecting the softness parameter to the dynamics, and also to the local devitrification process [5] the connection between the softness parameter and the structure is not clear. I will present a new measure of the structure of a liquid which is the softness of the mean-field caging potential developed by us earlier [2]. We find that this softness is sensitive to small changes in structure and can describe the dynamics of a wide range of systems [6]. We also find that the softness described in our study correlates with the ML study thus providing a theoretical framework for understanding the ML results. Finally, I will show that this softness parameter can be connected to the local mobility and should be considered a new order parameter that describes the small variation of the local structure in a supercooled liquid [7].*

[1] A. Banerjee, S. Sengupta, S. Sastry, and S. M. Bhattacharyya. Phys. Rev. Lett., 113, 225701 (2014).

[2] M. K. Nandi, A. Banerjee, C. Dasgupta and S.M. Bhattacharyya Phys. Rev. Lett., 119, 265502 (2017).

[3] F. P. Landes, G. Biroli, O. Dauchot, A. J. Liu, and D. R. Reichman, Phys. Rev. E 101, 010602 (2020).

[4] S. S. Schoenholz, E. D. Cubuk, and D. Sussman et al., Nat. Phys. 12, 469 (2016).

[5] D. Ganapathi, D. Chakrabarti, A. K. Sood, and R. Ganapathy, Nat. Phys. 17, 114 (2021).

[6] M. K. Nandi and S. M. Bhattacharyya, Phys. Rev. Lett. 126, 208001 (2021).

[7] M. Sharma, M. K. Nandi, S. M. Bhattacharyya arXiv:2108.00627v1