Séminaire

## Mardi 16 avril 2024 à 11h00

## Amphithéâtre Henri Benoît


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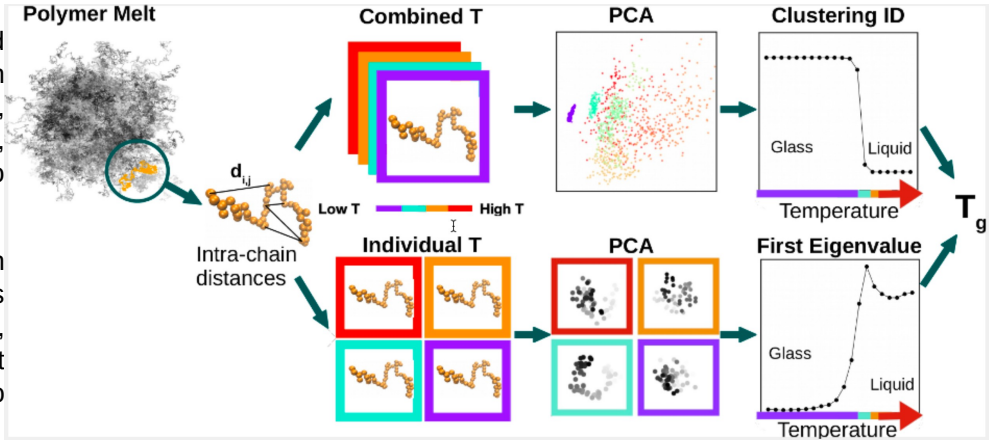
# Data-driven identification and analysis of the glass transition in polymer melts


On fast cooling, the dynamical properties of many polymer melts slow down exponentially, leading to a glassy state without any drastic change in static structure. Understanding the nature of glass transition, as well as precise estimation of the glass transition temperature for polymeric materials, remain open questions in both experimental and theoretical sciences. I will first talk about our new data-driven approach [1], which utilises the high-resolution details accessible through molecular dynamics simulation and considers the structural information of individual polymer chains. The method clearly identifies the glass transition temperature of polymer melts of semiflexible chains. By combining principal component analysis (PCA) and clustering (shown in the schematic), we identify glass transition temperature at the asymptotic limit even from relatively short-time trajectories, which just reach into the Rouse-like monomer displacement regime. More recently we applied this methodology to model all-atom acrylic paint systems [2]. In the end, I will talk about the data-driven identification of polymorphism in polymer crystals. Overall, I will discuss a general framework of utilising data-driven approaches to identify meaningful states in complex polymeric systems.



[1] Data-driven identification and analysis of the glass transition in polymer melts, Atreyee Banerjee, Hsiao-Ping Hsu, Kurt Kremer, Oleksandra Kukharenko, ACS Macro Lett., 12, 6, 679–684 (2023)

[2] Defining glass transition temperature in acrylic polymeric melts with machine learning methods, Atreyee Banerjee, Aysenur Iscen, Kurt Kremer, and Oleksandra Kukharenko J. Chem. Phys. 159, 074108 (2023)


*Les personnes souhaitant rencontrer A.Banerjee sont priées de prendre contact avec H.Meyer ou J.Baschnagel.*