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Ian Macmillan Ward Prize for Best Student Paper

Threading of ring polymers in gels and dense solutions

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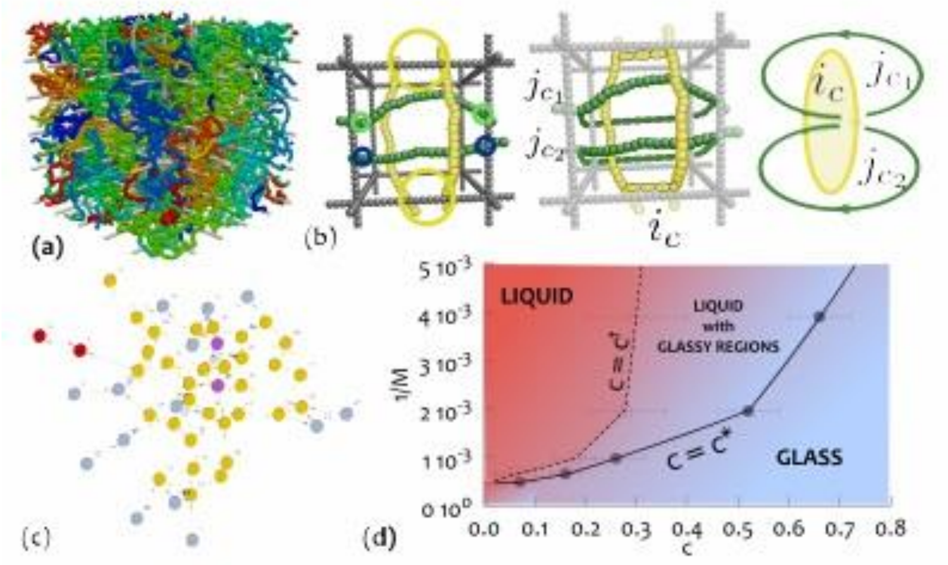
Ring polymers continue to present a challenge to the theoretical community as the polymers lack of ends represents a severe topological constraint on their conformations. Threadings between rings have been conjectured to play an important role in solutions of closed chains, from the work of Klein (Klein, Macromolecules 118 (1986)) to more recent ones (Kapnistos et al, Nat. Mater. 7 (2008) and Halverson et al, J. Chem. Phys. 134 (2011)), but always proved very elusive to directly detect and quantify. We perform large-scale Molecular Dynamics simulations of a concentrated solution of unknotted, unlinked rings in both, presence and absence of a background gel.

In the case in which the gel is present, we take advantage of its ordered architecture to introduce a rigorous algorithm to unambiguously identify local inter-ring threadings by measuring the linking of closed curves (Fig. (b)). We show that rings inter-thread through one another creating a systemspanning network of correlations (Fig. (c)) and that some of the threadings have a life-time that is at least comparable to that of the longest relaxation time of the chains.

In the case the gel is absent, it is currently impossible to unambiguously define a threading between two chains. On the other hand, their existence in a dense solution of rings is bound to affect the dynamics of the constituents. We therefore introduce a novel protocol to perturb the system and probe their presence in a dense solution of rings: we artificially freeze a fraction c of rings in the system. By increasing the length of the rings we observe that a smaller and smaller fraction of frozen rings is needed to induce a kinetic arrested state in the system (Fig. (d)), strongly suggesting the presence of extensive correlations that can eventually lead to a spontaneous vitrification in the limit of large rings.

We finally argue that these inter-ring interactions, or threadings, can explain most of the recent puzzling outcomes of experiments and simulations of systems of rings, and can contribute toward the understanding of the role of topology in systems of polymers.



(a) Snapshot of the system. (b) Representation of the threading detection algorithm indicating the closure construction that we employ. (c) Snapshot of the directed network of interpenetrating rings. (d) Liquid-glass phase diagram for a dense solution of rings M beads long where a fraction c of rings is artificially frozen.