

Searching the microscopic features responsible for an undercooled liquid behavior in charged rods

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Current Molecular Dynamics simulation results show that a fluid composed by rods with separated charges placed on the extremes exhibits typical behavior of an undercooled liquid provided that the charges are large enough¹. Thus, we have found that the orientation correlation functions changes dramatically when the charges on the extreme increase. Moreover, shear viscosity changes by several orders of magnitude with slight differences of temperature and also remarkable changes on the diffusion coefficient are observed. In this contribution we explore in a systematic way the appearance of this behavior by considering variations on the thermodynamic variables as temperature and density but also on the length of the rod and on a shifting of the charges respect to the geometric center. This study is based on our previous results about the correspondence between systems composed by linear molecular with point dipoles or with discrete charges².

The second element previously studied was the influence of the charge shifting along the molecular axis on the structure and thermodynamics of dipolar linear rods³. All these previous results refer to equilibrium properties but, as far as we are aware, no results about the dynamics of these systems and the appearance of a glass-like phase have been previously reported.

[1].-S.Lago, M.Cortada, J.A.Anta and S.Calero (to be published)

[2].- S.Calero, B.Garzón and S.Lago; *J.Chem.Phys.***118**, 11079-11091, (2003)

[3].- S. Lago, S.López-Vidal, B.Garzón, J.A.Mejías, J.A.Anta and S. Calero; *Phys.Rev.E* **68**,021201(1-4),(2003)