

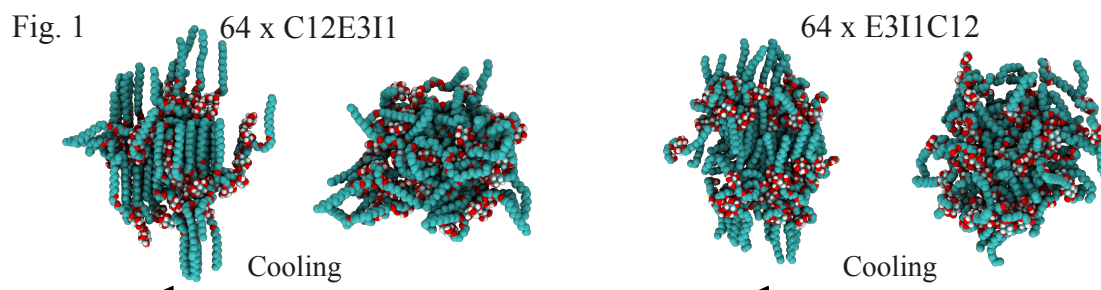
# Predicting Molecular Self Organisation in Sugar Based Liquid Crystals Using Grid Computing Facilities

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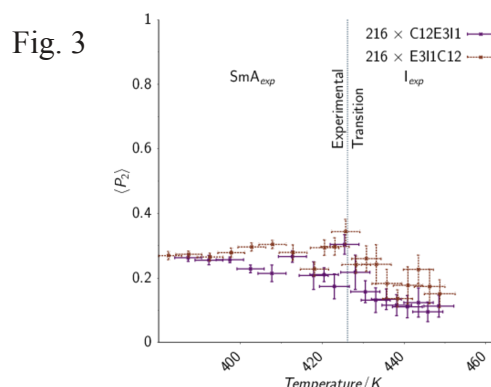
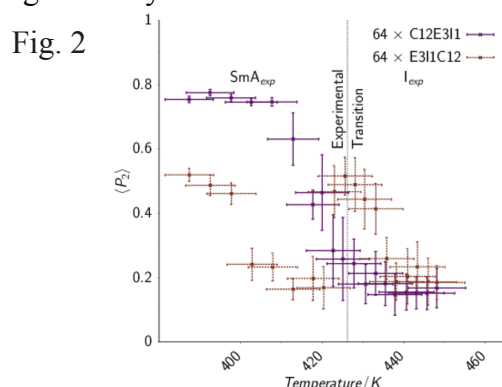
The prediction of transition temperatures of liquid crystalline compounds is a currently highly investigated topic in the field of materials sciences.[1] However, the simulation of bulk materials is a demanding research topic both scientifically and computationally.

Here, the self-organization of two sugar based model systems is discussed. Although both systems consist of an inositol moiety (I1), a dodecyl function (C12), and a triethoxy moiety (E3) only the combination C12E3I1 exhibits a liquid crystalline (SmA) phase in experimental findings while E3I1C12 transits directly from the isotropic to the crystalline phase.[2] Both systems have been MD-simulated with 64 molecules each, respectively, in a stepwise cooling approach (sampling time/temperature: 72 ns), cf. Fig. 1. The obtained trajectories are characterized by means of their nematic order parameter  $\langle P_2 \rangle$ .



The quite flexible alkyl and triethoxy chains lead to a high degree of freedom, which becomes more prominent in bigger simulation systems. Furthermore, the hydrogen bond interactions slow down the motility of the system in comparison to pure alkyl or aryl systems. In a simulation run with 64 molecules a self organization process became visible. Although a raise in order can be observed in both systems (C12E3I1 and E3I1C12) only the C12E3I1 system remains stable in its order while the E3I1C12 system destabilizes again (cf. Fig. 2).

These results were not reproduced with a system of 216 molecules and 72 ns sampling time (cf. Fig. 3). A possible explanation would be that the sampling time of the bigger system has to be significantly increased.



The calculations were achieved within the MoSGrid (Molecular Simulation Grid) project which aims to facilitate the access to high performance computational resources for chemical simulation purposes.[3]

[1] G. Tiberio, et al., *Chem. Phys. Phys. Chem.*, **2009**, 10, 125-136.

[2] a) G. Catanoiu, et al., *Langmuir* **2007**, 23, 12802-12805; b) G. Catanoiu, et al., *J. Colloid Interface Sci.* **2012**, 371, 82-88.

[3] MoSGrid is funded by the Federal Ministry of Education and Research under grant 01IG09006; <http://www.mosgrid.de/>