Structural Modification in Soft Matter Envisioned by Molecular Modeling

A. Soldera
Département de Chimie, Université de Sherbrooke, Sherbrooke (Québec), J1K 2R1 Canada

Soft matter, more specifically polymers and liquid crystals, offer some advantages comparing with inorganic materials: processing, low cost. Moreoever, their chemical structure can be easily modified. Nevertheless, a small change can have drastic effects on final properties. For instance, a difference in the configuration of PMMA, poly(methyl methacrylate), chain gives a variation of the glass temperature transition, T_g, of more than 60 °C ! Could then molecular modeling envision such variations ? In the affirmative, it provides a suitable tool to understand the reasons that give rise to such modification, and consequently, to design new compounds with optimal properties. Actually, to complete these two aims successfully molecular modeling has to be complementary with experimental data and theoretical background.

To illustrate these molecular modeling purposes, two examples are presented. The first example concerns the difference in T_gs between the two PMMA configurations. It will be shown that molecular modeling can represent such a variation. As a matter of fact, energetic analysis and microscopic investigations can be carried out to understand the glass transition phenomenon. The second example concerns more specifically the design of new ferroelectric liquid crystal compounds with optimal non-linear optical properties. In both examples, a stimulate interconnection of molecular simulation with theory and experimental data is presented.