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Ionic Conductivity in Discotic Liquid Crystals of hexa-*peri*-benzocoronenes (HBC) doped with lithium triflate (LiTf)

A. Pipertzis[1], K. Wunderlich[2], K. Müllen[2], G. Floudas[1]
[1]*Department of Physics, University of Ioannina, P.O. Box 1186, 451 10 Ioannina, Greece*
[2]*Max-Planck Institute for Polymer Research, D -55128 Mainz, Germany*

Abstract:

Discotic liquid crystals (DLCs) have attracted considerable interest because of their unique self-organization behavior into columnar superstructures[1]. Their self-assembly is driven by noncovalent intermolecular interactions favoring the π-stacking of aromatic cores.[2-4]Herein we explore the possibility of electronic and ionic conduction in model DLCs, in possible applications as Solid Polymer Electrolytes[5] in lithium ion batteries[6]. For this purpose we design a DLC of hexa-*peri*-benzocoronenes (HBC) with six chains of triethylene glycol dimethyl ether (TEG) doped with lithium triflate (LiTf) in three salt concentrations [EO]:[Li^+]=12:1, 8:1 and 3:1. The columnar organization ("hard nanophase") supports the electronic conductivity (i.e molecular wires[7-8]) whereas TEG functionalization ("soft nanophase") and addition of lithium triflate (LiTf) results in ionic conductivity. We have employed (a) differential scanning calorimetry (DSC) to investigate the thermal properties of DLCs, (b) X-ray scattering to determine the unit cell and the nanodomain structure, (c) dielectric spectroscopy (DS) to determine the ionic conductivity and the molecular dynamics and (d) rheology to determine the viscoelastic properties. The bulk HBC-TEG6 undergoes a low temperature phase transition from crystalline (Cr) phase to liquid-crystalline (LC) phase and a transition at higher temperatures due to the change of unit cell. The addition of lithium triflate (LiTf) stabilizes the high temperature unit cell and in addition organized into a superstructure that is detected in DSC, X-rays, DS and in rheology. The ionic conductivity is ≈ 3.6×10^{-6} S/cm at T= 363 K of the HBC-TEG6/LiTf with salt concentration [EO]:[Li^+]=3:1. Ionic conductivity of these composite systems is reduced by 2 decades in comparison to the respective TEG6/LiTf with the same salt concentration. Furthermore DS revealed that ion transport is coupled to the segmental dynamics.

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