Electronic Transport in Discotic Liquid Crystal Columns

L. Lever[1,2], R. J. Bushby[2,3] and R. W. Kelsall[1]

1. School of Electronic and Electrical Engineering
2. Centre for Self Organising Molecular Systems
3. School of Chemistry

University of Leeds, Leeds LS2 9JT, UK
email: r.w.kelsall@leeds.ac.uk

The has been much recent interest in conducting discotic liquid crystals for applications in chemical sensing and in molecular optoelectronic devices such as organic light emitting diodes and photodetectors. The most common discotic (disk-like) molecules, such as the those of the triphenylene and pthalocyanine families, comprise a flat, aromatic core to which are attached a number of alkyl side chains. The molecules exhibit strong self-organisation properties: the molecules stack, core on core, to form long columns and, on a surface, the columns themselves are arranged in a hexagonal close-packed array. The resulting film has highly anisotropic electronic properties, with the conductivity along the column axis being typically three orders of magnitude higher than that perpendicular to the columns.

Conduction along discotic molecular columns was originally assumed to be due to hopping transport. However, hole mobilities of the order of 1 $cm^2V^{-1}s^{-1}$ have been reported for columns formed from two complementary triphenylene species, which results in a higher degree of ordering than obtained from each single species alone. The mobility values for the highly ordered discotic columns also show a very weak temperature dependence. Both these points argue against a hopping transport mechanism. In this work we investigate the possibility of band transport in discotic molecular columns, by using a Monte Carlo simulation of hole transport in a 1-dimensional periodic array. The effect of different types of defects - including vacancies and dislocations – is investigated to determine the likely extent of disorder in the material based on the measured mobilities. A stochastic distribution of coherence lengths is used. Phonon scattering is also included, due to out-of-plane vibrations of the carbon-hydrogen bonds on the aromatic core, but is found to have a relatively small effect on the overall mobility.

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