Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Charge mobility of discotic mesophases of polyaromatic hydrocarbons: a multiscale quantum/classical study[1] DENIS ANDRIENKO, VALENTINA MARCON, KURT KREMER, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, JAMES KIRKPATRICK, JENNY NELSON, Department of Physics, Imperial College London, Prince Consort Road, London SW7 2BW, United Kingdom — Discotic liquid crystals form columnar phases, where the molecules stack on top of each other and the columns arrange in a regular lattice. The self-organization into stacks results in the one-dimensional charge transport along the columns. Using atomistic molecular dynamics (MD) simulations we study columnar discotic phases formed by various polyaromatic hydrocarbons. Combining Kinetic Monte Carlo and MD trajectories a correlation between the material morphology and charge mobility is then established. We are able to reproduce the trends and magnitudes of mobilities as measured by pulse-radiolysis time-resolved microwave conductivity technique.

[1]supported by DFG via IRTG between Germany and Korea. VM acknowledges AvH Foundation. JK acknowledges EPSRC.

Denis Andrienko
Max Planck Institute for Polymer Research,
Ackermannweg 10, 55128 Mainz, Germany

Date submitted: 02 Dec 2007 Electronic form version 1.4