

Abstract Submitted
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Charge mobility of discotic mesophases of hexabenzocoronene derivatives: a multiscale quantum/classical study of the effects of side chain substitution¹ 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 the solid and liquid crystalline columnar discotic phases formed by the alkyl-substituted hexabenzocoronene mesogens. Correlations between the molecular structure, packing, and dynamical properties of these materials are established. Combining Kinetic Monte Carlo and MD trajectories a correlation between the material morphology and charge mobility is then obtained. We are able to reproduce the trends and magnitudes of mobilities as measured by pulse-radiolysis time-resolved microwave conductivity technique.

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