Abstract Submitted
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Rational design of the shape and periphery of discotics: a synthetic way towards high charge carrier mobilities[1] DENIS ANDRIENKO, XINLIANG FENG, VALENTINA MARCON, WOJCIECH PISULA, Max Planck Institute for Polymer Research, JAMES KIRKPATRICK, Imperial College London, FERDINAND GROZEMA, TU Delft, KURT KREMER, KLAUS MÜLLEN, Max Planck Institute for Polymer Research — Conjugated materials offer the revolutionary prospect of producing semiconductor devices at low cost. The best to date discotics are built around the coronene unit and possess six fold symmetry. In the discotic phase six fold symmetric molecules stack with an average azimuthal twist of 30 deg, whereas the angle which would lead to the greatest electronic coupling and hence highest charge mobility is 60 deg. Here, a molecule with three fold symmetry and alternating hydrophilic/hydrophobic side chains is synthesized and X-ray scattering is used to prove the formation of the desired helical microstructure. Pulse radiolysis time resolved microwave conductivity measurements show that the material has indeed a very high mobility in the plastic crystalline phase, in the range of $0.1 - 0.2\,\mathrm{cm}^2/\mathrm{Vs}$. The physical structure of the assemblies of molecules are simulated using molecular dynamics. This, together with quantum chemical techniques, allows the computation of charge mobilities without fitting parameters. The calculations prove that mobility is still limited by structural defects and that a defect free assembly would lead to mobilities in excess of $10\,\mathrm{cm}^2/\mathrm{Vs}$.

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Denis Andrienko
Max Planck Institute for Polymer Research

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