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Charge transport in conjugated polymers: a multiscale picture[1]
VICTOR RUEHLE, Max Planck Institute for Polymer Research, JAMES KIRKPATRICK, Imperial College London, KURT KREMER, DENIS ANDRIENKO, Max Planck Institute for Polymer Research — A framework to study charge transport in conjugated polymers using realistic morphologies is developed. First, the atomistic force field is refined using first-principles calculations. Systematic coarse graining is then performed to extend simulation times and system sizes accessible to molecular dynamics simulations. Material morphologies are generated using the coarse grained and atomistic models. Finally, the charge mobility is obtained using temperature activated hopping picture for charge transport [1]. The framework is tested on neutral and oxidized polypyrrole with different structural ordering [2].

[1] J. Kirkpatrick, V. Marcon, J. Nelson, K. Kremer, D. Andrienko, Phys. Rev. Lett. 98, 227402 (2007)
[2] V. Ruehle, J. Kirkpatrick, K. Kremer, D. Andrienko, Phys. Stat. Solidi B, 245, 844 (2008)

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