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Autore	Kordt Pascal
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Sommario/riassunto	In the field of organic semiconductors researchers and manufacturers are faced with a wide range of potential molecules. This work presents concepts for simulation-based predictions of material characteristics starting from chemical stuctures. The focus lies on charge transport - be it in microscopic models of amorphous morphologies, lattice models or large-scale device models.An extensive introductory review, which also includes experimental techniques, makes this work interesting for a broad readership. Contents: Organic Semiconductor DevicesExperimental TechniquesCharge Dynamics at Dierent ScalesComputational MethodsEnergetics and Dispersive TransportCorrelated Energetic LandscapesMicroscopic, Stochastic and Device SimulationsParametrization of Lattice ModelsDrift-Diusion with Microscopic Link