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Investigation of a 3D-crosslinked nonconjugated Radical Polymer to Tune Electrical Conductivity

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Organic-based high-performance semiconductor research has attracted significant attention not long ago because of their promising performance. Since the morphology of the solution-processed conductive polymers, used in organic semiconductors, affects the intrinsic charge transport characteristics and mechanical properties, several strategies have been searched to control molecular ordering and alignment enhancing performance. Also, improving performance requires using a measurement technique for molecular orientation and a molecular dynamics simulation approach to predict electrical and mechanical properties.
Our work presents a protocol that adopts the four angles technique to provide an accurate measurement of molecular orientation and a Hamiltonian Monte Carlo simulation to investigate charge transport characteristics. The four angle technique offers precise information on the molecular orientation of selected molecules utilizing the alignment of the electric vector of the Polarised Infrared probing beam with the dipole oscillation corresponding to the absorbing frequency of a specific functional group. In contrast, the Monte Carlo simulation algorithm can generate polymeric molecular chains following a standard random walk controlled by Hamiltonian parametrized utilizing Ab Initio calculations. This simulation will depend on radical concentration, the distance between radicals, and radical orientation to the polymer backbone, allowing to investigate the effect of radical and defect densities on the formation of the percolation network, which supports designing conductive polymers with high conductivity.
Key Words:
Four Angle Approach, Organic-based high-performance semiconductor, Nonconjugated radical polymer, Monte Carlo Simulation, Hamiltonian parametrized utilizing Ab Initio calculations.

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