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Theoretical Modeling and Design of Organic Semiconductors with High Carrier Mobility[1] XIAO MA, CHANGGUA ZHEN, JOHN KIEFFER, University of Michigan, Ann Arbor — Charge transport in organic materials can be quite different from that in inorganic materials. The weak van der Waals interaction between organic molecules invalidates the band model used widely in inorganic materials. We have applied a multiscale hopping model based on Fermi's golden rule to study the carrier mobility in a pentacene single crystal structure. The pentacene single crystal adopts a herringbone stacking, which strongly limits the π-orbital overlap between neighboring molecules, resulting in poor charge carrier transfer and long-range mobility. To improve the charge transport performance of pentacene-related organic materials, we functionalize the pentacene with polyhedral oligomeric silsesquioxanes (POSS) cages to induce a parallel configuration. A higher theoretical carrier mobility is predicted based on using a combination of molecular dynamics, density functional theory calculations and kinetic Monte Carlo simulations. Accordingly, simulations constitute a cost-efficient means to derive design principle for materials with improved transport properties to be used in photovoltaic devices.

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