Mesoscale molecular network formation in amorphous organic materials

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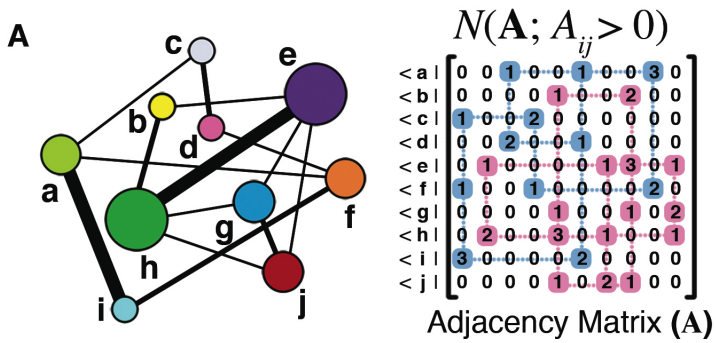
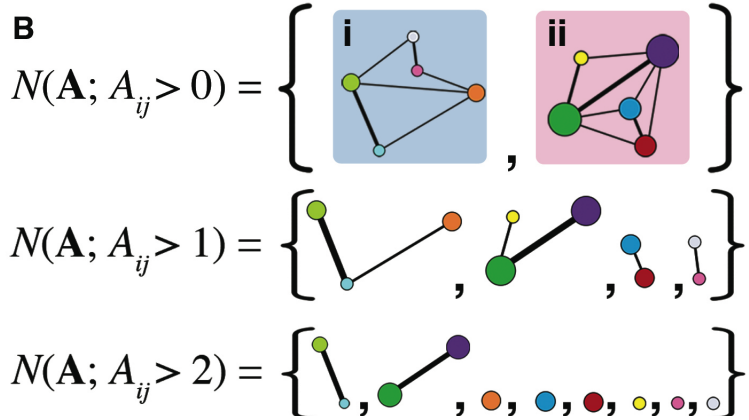
Graph Methodology for Understanding Mesoscopic Molecular Networks.

Sustainable progress in organic semiconductor design ultimately requires a quantitative predictive understanding of the way materials transport properties respond to structural disorder, a fact which is especially true for solution-processed organic photovoltaics. Combining molecular dynamics, electronic structure, and graph theoretical methodologies, **Savoie, Kohlstedt and Jackson** developed a novel means of analyzing the mesoscopic transport networks formed from commonly used organic photovoltaic acceptor materials (fullerenes and perylene diimiides).





A clear link was established between the success of mono and bis functionalized fullerenes and their ability to construct mesoscopically connected electrical networks over length scales of 10 nm, clearly demonstrating a direct correlation between network robustness and molecular topology (**Fig 1**). Additionally, this framework was utilized to show that solubilizing moieties play a large role in disrupting the molecular networks responsible for charge transport. This novel graph theoretic methodology provides both an improved understanding of the ability of a molecule to form transport networks based on single-molecule properties, as well as a quantitative means of screening a molecule's ability to form percolative electrical networks.

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