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Design of molecular sidechains to enhance thermal conductivity[1]

KIERAN MULLEN, DANIEL GLATZHOFER, Univ of Oklahoma — Higher thermal conductivity polymer composites would provide lighter and cheaper materials for large scale industrial applications as well as improve heat dissipation on the microscopic scale in electronics. Carbon nanotubes and graphene have high intrinsic thermal conductivity, but their large interface thermal resistance prevents their use in polymer composites. We investigate the design of molecular sidechains built from selectively chlorinated and/or fluorinated carbons which have the advantage of a higher linear mass density than an alkane chain and are expected to be quite stiff. We present results of a search for an optimal configuration of a sidechain consisting of a number of chlorinated carbon, fluorinated carbon, and simple hydrogenated carbon units that maximizes heat flow. This search will involve concepts from electron transport generalized to the study of phonon transport.

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