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Thermal and electrical conductivity of defective graphene: From grain boundaries to haeckelite[1] ZHEN ZHU, ZACHARIAS G. FTHENAKIS, DAVID TOMANEK, Michigan State University — We study the effect of structural defects on the electronic and thermal conductivity of graphene from first-principles calcluations. After optimizing defective structures using density functional theory, we describe ballistic charge transport using the non-equilibrium Green's function formalism and thermal transport using non-equilibrium molecular dynamics simulations. We find that both the electrical conductance G and thermal conductivity λ depend sensitively on the nature, concentration and arrangement of 5-7 and 5-8 defects, which may form grain boundaries in the honeycomb lattice of graphene or, at large concentrations, convert it to haeckelite. Lines of defects in graphene turn both σ and λ anisotropic. In a defective structure of graphene nanoribbons interconnected by haeckelite strips, the electrical conductance G increases, whereas the thermal conductivity is quenched by up to 1-2 orders of magnitude, mainly due to the reduced phonon mean free path. We conclude that defects play a profound role in the electrical and thermal transport of graphene.

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