Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Can graphene allotropes surpass the high thermal conductivity of graphene?[1] ZACHARIAS FTHENAKIS, ZHEN ZHU, DAVID TOMÁNEK, Michigan State University — Searching for materials with very high thermal conductivity, we explore the possibility that specific carbon allotropes may even surpass the high thermal conductivity of graphene and carbon nanotubes. We focus our study on graphene allotropes including 5-7 or 5-5-8 haeckelites with planar structure and sp^2 graphitic bonding. In contrast to graphene, these anisotropic systems should also conduct heat differently in different directions. Our computational studies use non-equilibrium molecular dynamics simulations based on the valence-bond force field parameterized by Tersoff and a Nose-Hoover thermostat to regulate the temperature. Whereas thermal conductivity of most haeckelite systems is reduced by an order of magnitude in comparison to graphene due to a lower phonon mean-free path, there is a distinct possibility that the isotropic thermal conductivity of graphene may be surpassed at least along particular directions in specific artificial haeckelite superstructures.

[1]Supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled "NSEC: Center for High-rate Nanomanufacturing".

Zacharias Fthenakis
Michigan State University

Date submitted: 02 Nov 2012 Electronic form version 1.4