

Abstract Submitted
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Thermal conductivity of partially hydrogenated graphene JEONG YUN KIM, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Graphene superlattices made with partial hydrogenation are of great interest and have been explored recently due to the enhanced tunability of electronic properties as a function of the hydrogenation pattern. However, the thermal transport properties of such materials have received little attention. In this work, we investigate the effects of 2D periodic patterns of hydrogen atoms on the thermal conductivity of partially hydrogenated graphene using classical molecular dynamics simulations and an Einstein relation. Our calculations show that the thermal conductivity of partially hydrogenated graphene varies substantially as a function of hydrogen coverage, periodicity, edge shape, and width of hydrogenated region compared to the bare graphene region. In addition, we show that the use of patterned 2D shapes of hydrogenation on graphene could lead substantially lower thermal conductivities that may be of interest for thermoelectric applications.

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