

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Effect of dopant distribution on thermal conductivity of  $C_{(1-x)}N_x$**   
YANG ZHOU, Fudan Univ — The thermal conductivities of nanoscale nitrogen doped graphene ( $C_{(1-x)}N_x$ ) with various nitrogen ratio and distribution is studied by performing nonequilibrium molecular dynamics. The thermal conductivity of randomly doped  $C_{(1-x)}N_x$  is found much smaller than that of the regular alloy when the dopant ratios are the same. Meanwhile, thermal conductivity of random alloys is dopant ratio sensitive while that of regular alloy is not. Interestingly, localization mode analysis indicates that the inequality of atoms under translation and inversion is responsible for the change of the thermal conductivity and a linear relationship between them is found. The results may provide a general guidance for phonon manipulation and thermal engineering in alloys.

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Date submitted: 06 Nov 2015

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