Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Phonons in Stabilized B or N doped graphene GIRIJA DUBEY, York College-CUNY, NY11451, SARITA MANN, POOJA RANI, VIJAY JINDAL, Department of Physics, Panjab University, Chandigrah 160014, India — Based on *Ab-initio* density functional perturbation theory, we have investigated various doped B and N based graphene sheets by raising their concentrations upto 50% of the host carbon. Although the doped structures seem to stabilize in 2-D configurations, but the resulting Phonon frequencies do not confirm the stability as the transverse modes above critical concentrations of B and N tend to result in negative eigenvalues. This essentially requires strained 2-D sheets when doped above such critical concentrations. We find the results of phonons and thermodynamics very interesting and attempt to report these in strained lattices. The motivation to do such a calculation results from our primary goal to address the issue of heat dissipation rate in the devices based on designable electronic and optical properties of such doped graphene reported already.

Girija Dubey
York College-CUNY, NY11451

Date submitted: 03 Nov 2015 Electronic form version 1.4