Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Designing Graphene-based Thermoelectric materials with Chemical Functionalization JEONG YUN KIM, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Graphene has been explored as a thermoelectric (TE) material recently due to its superior mobility and ambipolar nature. However, the extremely high thermal conductivity (κ) and only moderate Seebeck coefficient (S) make a graphene monolayer a highly inefficient TE material. Graphene superlattices made with chemical functionalization offer the possibility of tuning both the thermal and electronic properties via nano-patterning of the graphene surface. In this work, we investigate the effects of chemical functionalization on the thermoelectric transport properties of graphene using classical and quantum mechanical calculations. Our calculations show that chemical functionalization can control the power factor by changing the width of the pure graphene region and functionalization configuration, as well as κ depending on the functional groups and functionalization coverage. These results suggest that chemical functionalization could be an efficient route to designing graphene-based TE materials.

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Date submitted: 16 Nov 2012 Electronic form version 1.4