Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Thermal and Electronic Transport Properties of Graphene Nanoribbons with Defects JUSTIN HASKINS, Department of Chemical Engineering, Texas A&M University, ALPER KINACI, Department of Material Science, Texas A&M University, CEM SEVIK, TAHIR CAGIN, Department of Chemical Engineering, Texas A&M University — The interplay between graphene nanoribbon (GNR) structure and conductivity, both thermal and electrical, is probed with molecular dynamics and tight binding models. A variety of randomly oriented defects, vacancies and Stone-Wales, as well as edge terminations, zig-zag, armchair, and roughened, are studied in experimental sized systems (>100 nm long and >15 nm wide). It is found that GNR thermal conductivity responds similarly to edge roughness and moderate defect concentrations (0.0023) with a drastic reduction (81%) in lattice thermal conductivity, compared to pristine GNR value. Conversely, the presence of randomly oriented defects completely erodes the ballistic nature of the electrons, reducing conductance by two orders of magnitude, while edge roughened structures leave the electrical conductance intact.

Justin Haskins
Department of Chemical Engineering, Texas A&M University

Date submitted: 24 Nov 2010 Electronic form version 1.4