Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Thermally assisted self-trimming of graphene nanoribbon edges[1]
TENG YANG, DAVID TOMÁNEK, Michigan State University, SAVAS BERBER, Gebze Institute of Technology — Edge morphology is known to play a key role in the conductance of graphene ribbons. We use a combination of *ab initio* density functional total energy and molecular dynamics calculations to investigate thermally induced reconstruction occurring at graphene edges. The calculated total energy surfaces suggest that among all nanoribbon sites, atoms at edge defect sites require least energy to be displaced. At elevated temperatures, these atoms will primarily participate in diffusion and related processes at the edge that will gradually reduce the edge roughness and thus lower the edge energy. We explore various scenarios leading to such self-trimming of edges, including concerted migration processes and unravelling of chains at the edge. Close inspection of our results suggests that the preferential mechanisms and activation barriers for trimming of rough armchair and zigzag edges may be different. In selected scenarios, Joule heating of nanoribbons may not only straighten rough edges, but also modify the preferred edge morphology.

[1]Supported by NSF NIRT grant ECS-0506309 and NSF NSEC grant EEC-425826.

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Date submitted: 30 Nov 2008 Electronic form version 1.4