Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Topological defects in graphene: dislocations and grain boundaries[1] OLEG YAZYEV, STEVEN LOUIE, UC Berkeley and LBNL — Topological defects in graphene, dislocations and grain boundaries, are still not well understood despites the considerable number of experimental observations. We introduce a general approach for constructing dislocations in graphene characterized by arbitrary Burgers vectors as well as grain boundaries, covering the whole range of possible misorientation angles. By using ab initio calculations we investigate thermodynamic, electronic and transport properties of grain boundaries, finding energetically favorable large-angle symmetric configurations, strong tendency towards out-of-plane deformation in the small-angle regimes, pronounced effects on the electronic structure, and two distinct behaviors in the electronic transport - either perfect reflection or high transparency for low-energy charge carriers depending on the grain boundary structure. Our results show that dislocations and grain boundaries are important intrinsic defects in graphene which may be used for engineering graphene-based functional devices.

[1]Supported by NSF Grant No. DMR07-05941, US DOE Cont. No. DE-AC02-05CH1123 and Swiss NSF Fellowship PBELP2-123086. Computer resources from NERSC and NICS.

Oleg Yazyev
UC Berkeley and LBNL

Date submitted: 18 Nov 2009 Electronic form version 1.4