

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Formation of defect structures on graphene and CNTs: Effect of sulphur insertion¹ OGUZ GULSEREN, RASIM OVALI, GOKCE KUCUKAYAN, ERMAN BENGU, Bilkent University — Motivated from the possible mechanisms behind the junction formation on carbon nanotubes (CNTs), we investigated various defect structures of graphene by using planewave pseudopotential calculations based on density functional theory. The investigated defect structures, single or double vacancies, Stone-Wales defects, 4-5-7-8 rings of carbon, and combinations of these rings, are formed within large graphene nanoribbons where edges are saturated by hydrogen atoms. After geometry optimization, the cohesive and formation energies are calculated from corresponding total energies. For point defects, Stone-Wales, single 8-ring and single 7-ring type defect structures, the relaxed structures remain almost planar with a little local distortion; therefore, these structures might not be an appropriate initial structure for Y-junction formation on CNTs. However, the single 4-ring or various 5-ring (single, double and triple 5-rings) defects have highly curved final geometries and it becomes sharper from single to triple ring structures. Hence, these type of defect structures are good initial structure candidates for junction formation on CNTs. Then, the effects like insertion of sulphur that might lead such defect structures on graphene are investigated and discussed in detail.

¹This work is supported by TUBITAK under Grant No: 107T720.

Oguz Gulseren
Bilkent University

Date submitted: 20 Nov 2009

Electronic form version 1.4