Abstract Submitted
for the 4CF13 Meeting of
The American Physical Society

Ab Initio Study of Graphene Functionalized with Benzyne[1] SANJIV JHA, IGOR VASILIEV, New Mexico State University, IGOR MAGEDOV[2], LILIYA FROLOVA, NIKOLAI KALUGIN, New Mexico Tech — The electronic and structural properties of carbon nanomaterials can be affected by chemical functionalization. We apply *ab initio* computational methods based on density functional theory to study the covalent functionalization of graphene with benzyne. Our calculations are carried out using the SIESTA electronic structure code combined with the generalized gradient approximation for the exchange correlation functional. The calculated binding energies, densities of states, band structures, and phonon frequencies of graphene functionalized with benzyne are analyzed in comparison with the available experimental data. Our calculations show that the reactions of [2+2] and [2+4] cycloaddition of benzyne to the surface of pristine graphene are exothermic with the binding energies of -0.73 eV and -0.58 eV, respectively.

[1]Supported by NSF CHE-1112388. NSF ECCS-0925988, NIH-5P20RR016480-12 and NIH- P20 GM103451
[2]Deceased

Sanjiv Jha
New Mexico State University

Date submitted: 21 Sep 2013 Electronic form version 1.4