

Name

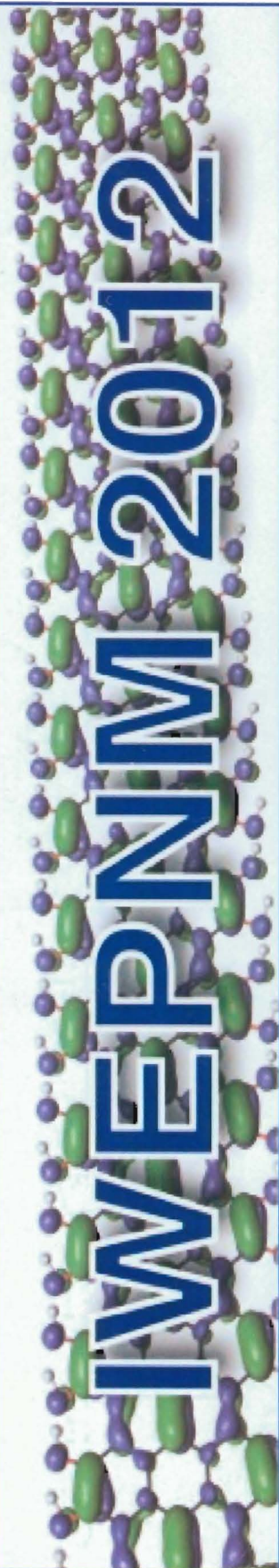
HUCZKO A

XXVIth
International
Winterschool
on
Electronic
Properties
of
Novel
Materials
Molecular
Nanostructures

Program

Hotel Sonalp
Kirchberg
Tirol
Austria

3-10 March, 2012



conduction for one growth condition to relatively low resistivity and little or no gate effect for the other growth condition. It is suggested that the latter result is due to a high density of surface states leading to doping past the Mott transition.

MON 24

Fast and efficient combustion synthesis route to produce exfoliated graphite

Agnieszka Dabrowska¹, Andrzej Huczko¹, Sławomir Dyjak²

¹Department of Chemistry, Warsaw University, 02-093 Warsaw, Poland

²Institute of Chemistry, Military University of Technology, 00-908 Warsaw, Poland

Micromechanical exfoliation produces graphene flakes from the layered material graphite. As the wet chemistry protocol, with the intermediate graphite oxide formation, is quite involving [1], we report the exploratory study on simple one-step chemical synthesis of exfoliated graphite via a combustion synthesis route. The different solid carbonates could be atomized upon reducing in solid phase [2]. The formed carbon elemental coalesced towards 1D nanocarbons. Recently, such processing was extended into the direct heterogeneous, high-pressure reduction of gaseous carbon oxides to elements (CO₂, CO) with Li, Mg, Ca, and other strong reducers in a modified calorimetric bomb [3]. The products were chemically purified. The morphology identification of produced layered carbon was done by XRD, SEM, TEM, Raman spectroscopy.

[1] M. Inagaki et al., *J. Phys. Chem. of Solids*, 675, 133-137 (2004)

[2] A. Dabrowska et al., *Phys. Status Solidi B*, 248, 2704-2707 (2011)

[3] A. Huczko et al., *J. Mater. Res.*, in print (2011)

This project is co-financed by the European Regional Development Fund within the Innovative Economy Operational Program 2007-2013, No.UDA-POIG.01.03.01-14-07108-06

MON 25

Equilibrium Torsion in Chiral Carbon Nanotubes

Milan Damjanovic¹, Natasa Lazic¹, Tatjana Vukovic¹, Ivanka Milosevic¹

¹NanoLab, Faculty of Physics, University of Belgrade, Belgrade

The proposal [1] of slight twist with respect to the rolled up configuration in chiral single-walled carbon nanotubes is recently numerically justified [2]. Only dynamical models supporting full helical symmetry (monomer becomes minimal repeating component) can show this effect, while standard DFT assume translational periodicity.

Here we present convincing evidence for the effect: very similar dependence of the torsion angle of the tube diameter (rapid decrease) and chiral angle within several dynamical models like pairwise harmonic potential, Brenner potential based molecular dynamics, and DFTB. Also, we give indirect justification of torsion using full DFT code SIESTA.