Modelling of Polymer-SWNT Systems: Selectivity Studies on Solubilizers for Carbon Nanotubes

Livia N. Glanzmann
Duncan J. Mowbray
Angel Rubio

POCAONTAS 1st Summer School, Ventotene (Italy)
2nd of June 2014
INTRODUCTION

PROJECTS (Results and Goals):

Modelling of the PFO-BPy polymer:
Method of periodically repeating monomer units

Modelling of monomer-SWNT System

Testing polymer series on selective behavior
(Técnico Lisboa, Julius-Maximilians-Universität Würzburg)

Modelling of carbon nanotubes using graphene
Photoluminescence mapping of PFO-BPy/SWNTs film on ITO electrodes [1].

Modelling of polymer-SWNT hybrid system

side chains?

repetition units?
Modelling of the PFO-BPy polymer: Method of periodically repeating monomer units

Linear response TD-DFT absorption spectra and average electron and hole densities of PFO-BPy Oligomers.
Modelling of the PFO-BPy polymer: Method of periodically repeating monomer units
Modelling of the PFO-BPy polymer: Method of periodically repeating monomer units

Py-PFO-Py
Modeling of hybrid system

Py-PFO-PY Monomer adsorbed on a 6,6-SWNT.
Testing polymer series on selective behavior
(Técnico Lisboa, Julius-Maximilians-Universität Würzburg)
Modelling of carbon nanotubes using graphene
Modeling of carbon nanotubes using graphene
Summary

Octyl $\rightarrow$ ethyl
Polymer $\rightarrow$ monomer
tube $\rightarrow$ graphene sheets

hybrid system
screen different polymers
Thank You!!