Electronic structure calculation of carbon structures with NEMO5 interfaced with Rappture

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ABSTRACT

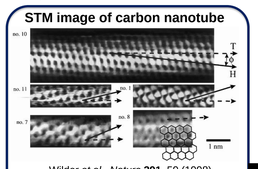
In a world looking to expand its technology, it is necessary to understand and implement materials that will allow such development to continue at a fast pace. Carbon based structures, such as, nanotubes (CNT) and nanoribbons (GNR) are amongst those materials due to its high conductivity and ability to be malleable which allows the material to be incorporated into complex structures. With this in mind it is important to know the material, transport properties of carbon structure by simulation. Although several tools on CNT and GNR are already deployed in nanoHUB, it is necessary in the long term to replace with maintainable and flexible simulation tool. In this work, we initiated implementing Rappture interface that loads a general nanoelectronic modeling tool, NEMO5, a simulation tool that is currently being developed by Network for Computer Technology (NCN) at Purdue. Along with NEMO5 it is necessary to implement a wrapper code in MATLAB format that serves as intermediary between NEMO5 and the rapid application structure (Rappture) that is currently used by the nanoHUB website. The wrapper reads data from Rappture GUI and generates input file for NEMO 5 and processes the simulation results in Rappture GUI display format. As a result, we benchmarked and demonstrated the unit cell and band structures of CNT with different chirality. Since NEMO5 is still under development, we expect to expand this work to show electronic structures of GNR's with advanced band models and add quantum transport in near future.

OBJECTIVE

- Understand the basic physics of carbon nanotubes (CNT) and graphene nanoribbons (GNR)
- Familiarize with the previous tool CNTBands in nanoHUB and the new engine NEMO 5 for future replacement
- Develop an initial Rappture framework that covers from electronic structure to quantum transport model for carbon base transistors

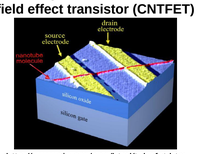
Physical structure / device

STM image of carbon nanotube



Wilder *et al.*, *Nature* **391**, 59 (1998)

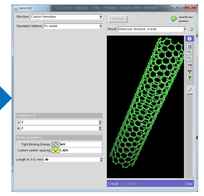
STM image of carbon nanotube field effect transistor (CNTFET)



http://www.aip.org/png/html/tubefet.htm

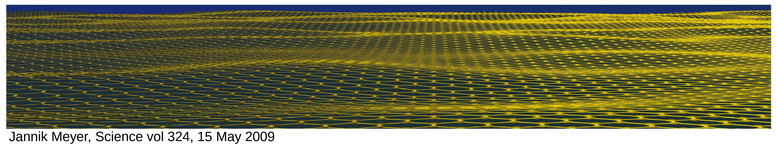
Theory / development

nanHUB deployment for research/education



MOTIVATION

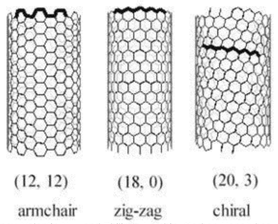
- Increased interests on Carbon materials
  - ✓ Research
  - ✓ Industry
- Emerging knowledge of CNTs
- Chemical sensing capabilities
- Remarkable quantum transport properties
- Several undiscovered capabilities



Jannik Meyer, Science vol 324, 15 May 2009

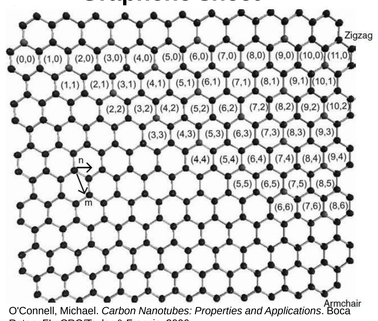
THEORY

- Carbon nanotube is formed from graphene ribbon
- Dependent on chiral indices
- Each structure has unique properties
- Applied to different fields
  - ✓ Used in electronics
  - ✓ Used in sensors



Popov, Valentin N. ., and Philippe Lambin. *Carbon Nanotubes*. Dordrecht: Springer, 2006.

Graphene sheet

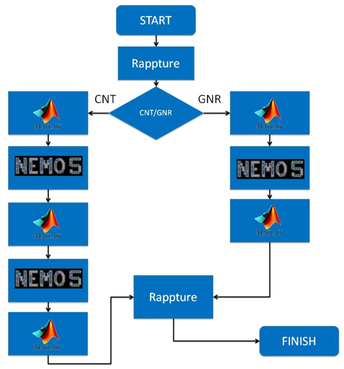


O'Connell, Michael. *Carbon Nanotubes: Properties and Applications*. Boca Raton, FL: CRC/Taylor & Francis, 2006.

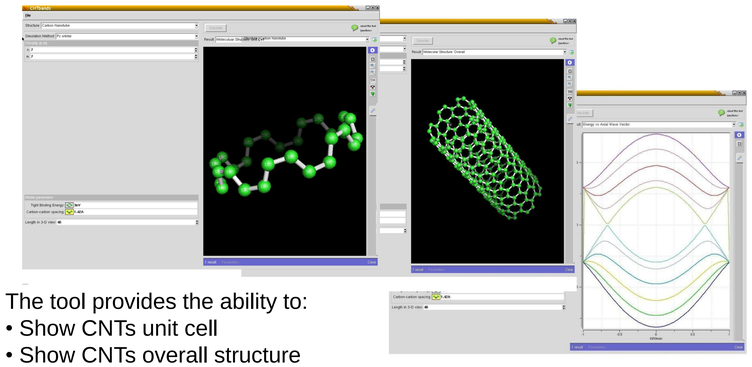
Carbon nanotubes with Different chirality

METHODOLOGY

The project consisted of integrating three different programming tools into an easy enough system that anyone could use. The main process was establishing a proper communication between **N**ano**E**lectronics **Mo**deling (NEMO5) and the **R**apid **app**lication infrastruc**ture** tool (Rappture). This communication was achieved by creating a MATLAB code which creates and manages the information necessary for the communication to exist. It first gathers the information given by the user and creates an input deck which holds the information of the structure along with those parameters given by the user. This input deck then runs the NEMO5 simulation. When the simulation is completed several files are created. Once again the MATLAB code comes into action by analyzing and interpreting all these new files. It then properly processes the information required to correctly display the information back to Rappture.



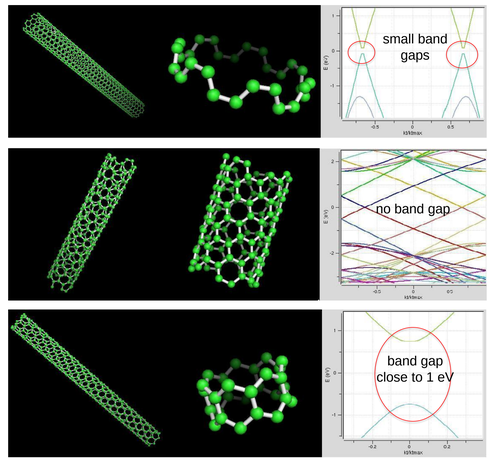
RESULTS



The tool provides the ability to:

- Show CNTs unit cell
- Show CNTs overall structure
- Simulate metallic and semiconducting structures
- Generate the band gap of GNRs and CNTs
- Give a copy of NEMO 5 input deck
- Generates an output log with several calculations
- Information of nanotube diameter, circumference and chiral angle

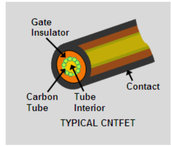
RESULTS



- Different material configurations have different properties
  - ✓ Semiconducting
  - ✓ Conductive
- Band gaps helps differentiate between materials
- Used for:
  - ✓ Transistors (semiconductor)
  - ✓ Wire (metallic)

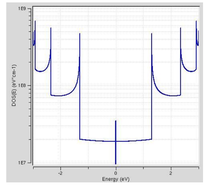
CONCLUSION

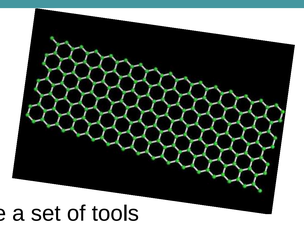
- Understand and analyze CNTs and GNRs
- Allow others to access this kind of information
- Leave an initial framework for future implementations of the quantum and electronic transport of carbon based transistors



FUTURE WORK

- Implement graphene nanoribbon
- Add density of states of both CNTs and GNRs





- Complete a set of tools that will allow user to simulate carbon based transistors

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4. O'Connell, Michael. *Carbon Nanotubes: Properties and Applications*. Boca Raton, FL: CRC/Taylor & Francis, 2006.