NanoCap Guide & Documentation

1 Introduction

NanoCap provides both libraries and a standalone application for the construction of capped nanotubes of arbitrarily chirality and fullerenes of any radius. Structures are generated by constructing a set of optimal dual graph topologies which are subsequently optimised using a carbon interatomic potential. Combining this approach with a GUI featuring 3D rendering capabilities allows for the rapid inspection of physically sensible structures which can be used as input for molecular simulation.
The NanoCap source and builds for different platforms can be found at:
`http://sourceforge.net/projects/nanocap/`

2 Fullerenes

3 Nanotubes

Although NanoCap was designed to produce fullerenes and cap nanotubes, isolated nanotubes can be constructed. These can be either finite in length or periodic along the axial direction.
A nanotube is constructed via:
File–>New Structure–>Single Structure
them click *Nanotube* from the popup menu.

3.1 Finite tubes

Finite tubes are simply constructed as close to the user defined length as possible. This length is defined in the **Calculations–>Input** options.

3.2 Periodic tubes

Periodic tubes are constructed using a user defined number of unit cells in the z direction. The number of unit cells can also be found in the **Calculations–>Input** options.
The nanotube will be associated with a *periodic length* which can be found in the **Information** options tab. This will be required by simulation software if the nanotube is to be used in a periodic simulation.

4 Capped Nanotubes

5 Force Fields

5.1 Dual Lattice Force Fields

Currently, only one force field is implemented to optimise a structure's dual lattice. The total energy of a system is given by the sum of pair interaction energies:

$$\phi = \sum_{i=1}^{N_D} \sum_{j=i+1}^{N_D} \frac{1}{|\mathbf{r_i} - \mathbf{r_j}|}$$

6 Optimisation

7 Scientific Publications

There are two papers associated with the theory and implementation of NanoCap. If NanoCap is used in your work, please cite the following:

1. **Generalized method for constructing the atomic coordinates of nanotube caps**
   M. Robinson, I. Suarez-Martinez, and N. A. Marks *Phys. Rev. B 87, 155430*

   Abstract:

   A practical numerical method for the rapid construction of nanotube caps is proposed. Founded upon the notion of lattice duality, the algorithm considers the face dual representation of a given nanotube which is used to solve an energy minimization problem analogous to The Thomson Problem. Not only does this produce caps for nanotubes of arbitrary chirality, but the caps generated will be physically sensible and in most cases the lowest energy structure. To demonstrate the applicability of the technique, caps of the (5,5) and the (10,0) nanotubes are investigated by means of density-functional tight binding (DFTB). The calculation of cap energies highlights the ability of the algorithm to produce lowest energy caps. Due to the preferential construction of spherical caps, the technique is particularly well suited for the construction of capped multiwall nanotubes (MWNTs). To validate this proposal and the overall robustness of the algorithm, a MWNT is constructed containing the chiralities (9,2)@(15,6)@(16,16). The algorithm presented paves the way for future computational investigations into the physics and chemistry of capped nanotubes.

   url: `http://journals.aps.org/prb/abstract/10.1103/PhysRevB.87.155430`

2. **NanoCap: A Framework for Generating Capped Carbon Nanotubes and Fullerenes**
M. Robinson and N. A. Marks *Com. Phys. Comm 2014*

Abstract:

NanoCap provides both libraries and a standalone application for the construction of capped nanotubes of arbitrarily chirality and fullerenes of any radius. Structures are generated by constructing a set of optimal dual graph topologies which are subsequently optimised using a carbon interatomic potential. Combining this approach with a GUI featuring 3D rendering capabilities allows for the rapid inspection of physically sensible structures which can be used as input for molecular simulation.

url: *tba*