

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*

then click *Nanotube* from the popup menu.

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.

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.