SYNOPSYS®

Carbon NanoTube Modeling with QuantumATK

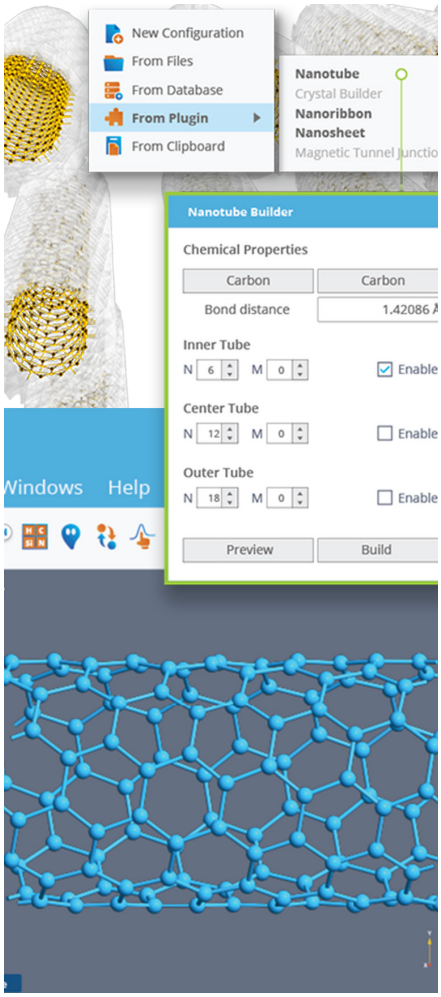
QuantumATK is a complete and fully integrated software suite for atomic-scale modeling of materials, nanostructures, and nanoelectronic devices, professionally engineered using state-of-the-art scientific and software-engineering methods. It combines the power of a Python scripting engine with the ease-of-use provided by an intuitive NanoLab graphical user interface (GUI). All simulation engines share a common infrastructure for analysis, ion dynamics, and parallel performance techniques.

Nanostructures with QuantumATK

Carbon nanotubes can be pictured as sheets of graphite rolled up into tubes. Their unique mechanical and electronic properties have been the subject of intense study both experimentally and theoretically, ever since their discovery (Sumio Iijima in 1991).

QuantumATK employs special algorithms which substantially improve the numerical performance when studying transport properties of nanotubes and other "long" systems, and excellent agreement has been obtained between experiments and calculations.

It contains instruments for constructing nanotubes and aligning them with a central scattering region, making it an ideal environment for transport studies in carbon nanotubes. One can for instance consider the resistance and capacitance of metal-nanotube or nanotube-nanotube contacts, or study electron field emission from carbon nanotubes.



Easy-to-Use Nanostructure Builders

- Builders for nanotubes, nanowires, nanoribbons, and nanosheets
- Builders for icosahedron and spherical nanoparticles
- Wulff construction tool for building nanoparticles with minimal surface energy
- Rich documentation system with many tutorials and instructions

Since 2006, over 2650 scientific articles have been published using QuantumATK. The software is used by over 400 research groups at leading universities, labs, and in the electronics industry around the world.

Synopsys
QuantumATK Team
Fruebjergvej 3
DK-2100 Copenhagen
DENMARK

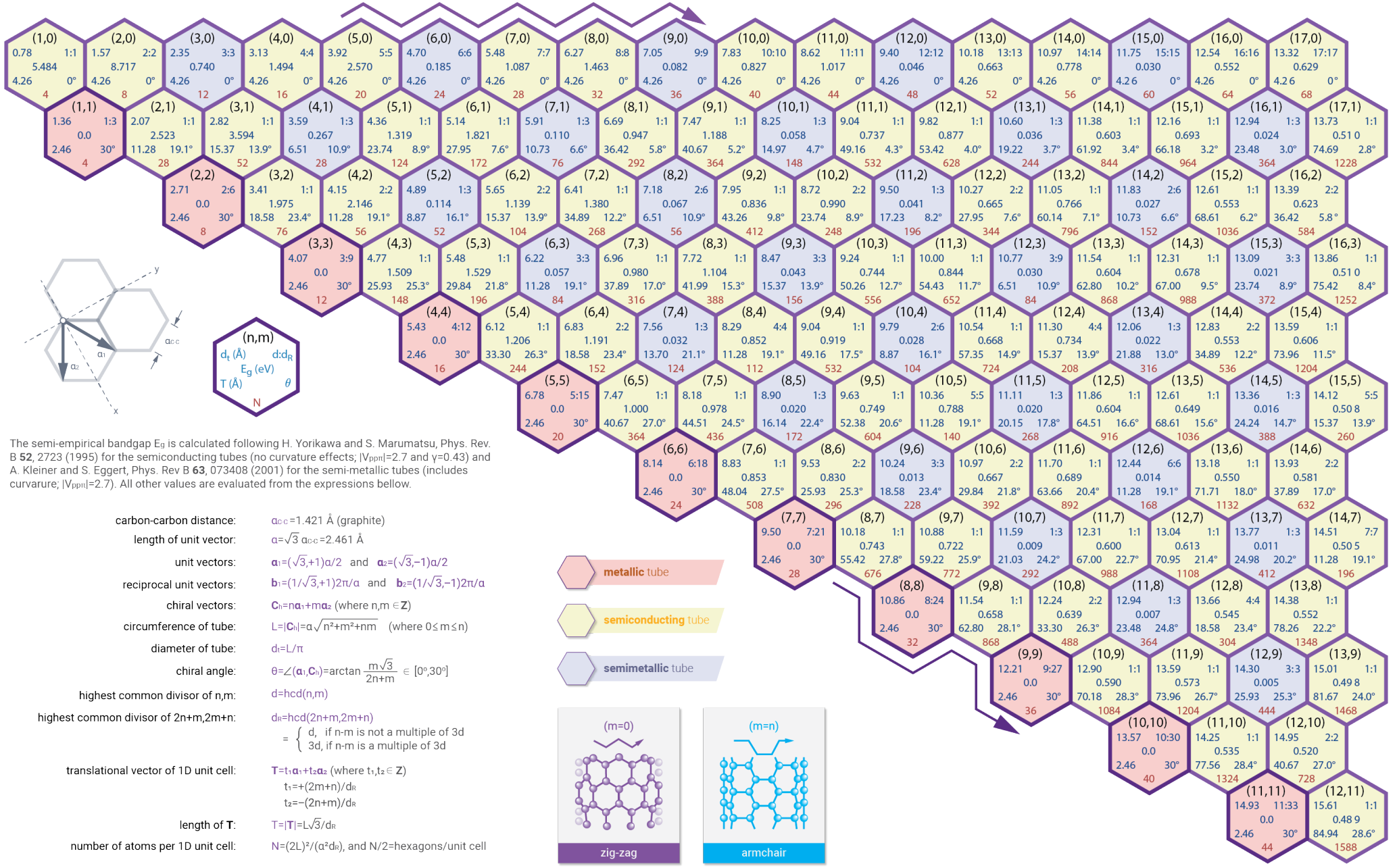
www.synopsys.com/quantumatk
quantumatk@synopsys.com
+45 333 32 300

SYNOPSYS®

SYNOPSYS®

Periodic Table of Carbon Nanotubes

www.synopsys.com/quantumatk
quantumatk@synopsys.com



The semi-empirical bandgap E_g is calculated following H. Yorikawa and S. Marumatsu, Phys. Rev. B **52**, 2723 (1995) for the semiconducting tubes (no curvature effects; $|V_{ppπ}|$=2.7 and γ=0.43) and A. Kleiner and S. Eggert, Phys. Rev B **63**, 073408 (2001) for the semi-metallic tubes (includes curvarure; $|V_{ppπ}|$=2.7). All other values are evaluated from the expressions bellow.

carbon-carbon distance:	$a_{c\text{-}c}$ =1.421 Å (graphite)
length of unit vector:	$a=\sqrt{3}\,a_{c\text{-}c}$=2.461 Å
unit vectors:	$\mathbf{a}_1=(\sqrt{3},+1)a/2$ and $\mathbf{a}_2=(\sqrt{3},-1)a/2$
reciprocal unit vectors:	$\mathbf{b}_1=(1/\sqrt{3},+1)2\pi/a$ and $\mathbf{b}_2=(1/\sqrt{3},-1)2\pi/a$
chiral vectors:	$\mathbf{C}_h=n\mathbf{a}_1+m\mathbf{a}_2$ (where n,m ∈ **Z**)
circumference of tube:	$L=\lvert\mathbf{C}_h\rvert=a\sqrt{n^2+m^2+nm}$ (where $0\le m\le n$)
diameter of tube:	$d_t=L/\pi$
chiral angle:	$\theta=\angle(\mathbf{a}_1,\mathbf{C}_h)=\arctan\frac{m\sqrt{3}}{2n+m}\in[0°,30°]$
highest common divisor of n,m:	$d=hcd(n,m)$
highest common divisor of 2n+m,2m+n:	$d_R=hcd(2n+m,2m+n)$ = { d, if n-m is not a multiple of 3d; 3d, if n-m is a multiple of 3d
translational vector of 1D unit cell:	$\mathbf{T}=t_1\mathbf{a}_1+t_2\mathbf{a}_2$ (where $t_1,t_2\in$ **Z**) $t_1=+(2m+n)/d_R$ $t_2=-(2n+m)/d_R$
length of **T**:	$T=\lvert\mathbf{T}\rvert=L\sqrt{3}/d_R$
number of atoms per 1D unit cell:	$N=(2L)^2/(a^2d_R)$, and N/2=hexagons/unit cell