Electronic Supplementary Material (ESI) for Nanoscale.

#Supplementary materials: MAPLE program
#Carbon nanotubes sorting due to commensurate molecular wrapping by Olga V. Konevtsova, Daria S. Roshal, Vladimir P. Dmitriev and Sergei B. Rochal
#Calculation of geometric parameters for possible nanotube coatings. Equations (4-7) from the Paper are applied. The results presented in Tables 1 and 2 were obtained using this program.

restart;
#setting the direction vector $\boldsymbol{S} = \langle h, k \rangle$

$h := -\frac{2}{3}$: $k := \frac{7}{3}$: *#selected indexes correspond to the vector **S_1** , see section 'General approach to the SWCNT selection...'.*

#distance between the tube and the coating
$dist := 0.34$:
#distance between positions of neighboring carbon atoms
$a0 := 0.142$:
#setting the path to the file where the results are written
ff := *fopen*("D:\\rez.txt", *WRITE*) :
#output of the table header
fprintf (*ff*, " n   m   d   Ns   Dz   S   T   alpha\n") :

#iterate over all possible indices of nanotubes
for *n* **from** 0 **to** 20 **by** 1 **do**
for *m* **from** 0 **to** 20 **by** 1 **do**
if $((m + n) > 1)$ **then**

$Q := \mathrm{sqrt}(m^2 + m \cdot n + n^2)$:

#nanotube diameter

$d := evalf\left(\frac{Q}{\mathrm{Pi}} \cdot a0 \cdot \mathrm{sqrt}(3)\right)$;

#number of molecules per one loop of the helix (see formula (5) in the Paper)

$Ns := evalf\left(\frac{2(m^2 + m \cdot n + n^2)}{((2n + m) \cdot h + (2m + n) \cdot k)}\right)$:

*#projection of the vector **S** on the tube axis*

$Sz := \frac{\mathrm{sqrt}(3) \cdot (-m \cdot h + n \cdot k)}{2 \cdot Q}$:

#pitch of the helix

$Dz := evalf(Ns \cdot Sz \cdot \mathrm{sqrt}(3) \cdot a0)$;

#side length S of coating supercells

$S := evalf\left(\mathrm{sqrt}\left(Sz^2 \cdot 3 \cdot (a0)^2 + \frac{(Q \cdot \mathrm{sqrt}(3) \cdot a0 + 2 \cdot \mathrm{Pi} \cdot dist)^2}{Ns^2}\right)\right)$;

#integer part of the number Ns

$Z := \mathrm{trunc}(Ns)$;

#side length T (T' in the paper) of coating supercells

$T := \mathrm{sqrt}\left(\frac{(Q \cdot \mathrm{sqrt}(3) \cdot a0 + 2 \cdot \mathrm{Pi} \cdot dist)^2}{Ns^2} (\mathrm{frac}(Z - Ns + 1))^2 + (Dz + Sz \cdot \mathrm{sqrt}(3) \cdot a0 \cdot (\mathrm{frac}(Z - Ns + 1)))^2\right)$;

#calculating projections for basic nanotube spiral wrapped along the <1, −1> direction

$$Ap := evalf\left(\frac{((2\,n+m)-(2\,m+n))}{2\cdot Q^2\cdot \mathrm{sqrt}(3)\cdot a0}\cdot(Q\cdot \mathrm{sqrt}(3)\cdot a0+2\cdot \mathrm{Pi}\cdot dist)\right):$$

$$Az := evalf\left(\frac{\mathrm{sqrt}(3)\cdot(-m-n)}{2\cdot Q}\right):$$

*#calculating T'= ⟨Tp, Tz⟩ projections onto the vector **P** and tube axis*

$$Tp := evalf\left(\frac{(Q\cdot \mathrm{sqrt}(3)\cdot a0+2\cdot \mathrm{Pi}\cdot dist)}{Ns}\cdot(\mathrm{frac}(Z-Ns+1))\right):$$

$$Tz := evalf(Dz+Sz\cdot \mathrm{sqrt}(3)\cdot a0\cdot(\mathrm{frac}(Z-Ns+1))):$$

*#angle α between the vector **T '** and the direction vector of the basic nanotube spiral*

$$\mathrm{alpha} := 180 - evalf\left(\frac{\arccos\left(\frac{(Az\cdot Tz+Ap\cdot Tp)}{\mathrm{sqrt}(Az^2+Ap^2)\cdot \mathrm{sqrt}(Tz^2+Tp^2)}\right)\cdot 180}{\mathrm{Pi}}\right);$$

#printing the geometrical parameters for limited values of the diameter

if $(d > 0.47)$ **and** $(d < 1.22)$ **then**
fprintf (*ff*,
"%2.0f %2.0f %2.2f %2.2f %2.2f %2.2f %2.2f %2.2f\n", *n*, *m*, *d*, *Ns*, *Dz*, *S*, *T*, Re(alpha));
fi;**fi**;
od;
od;
fclose(*ff*) :