In[1]:=
```
Print["  The source of the data of the manuscript                    "];
Print[" Structure and energetics of carbon, hexagonal boron nitride, "];
Print[" and carbon/hexagonal boron nitride single-layer and bilayer nanoscrolls "];
Print[" / A.I. Siahlo, N.A. Poklonski, A.V. Lebedev, I.V.
    Lebedeva, A.M. Popov, S.A. Vyrko, A.A. Knizhnik, Yu.E. Lozovik "];
Print[" // Phys. Rev. Materials.— 2018.— V. 2, № 3.— P. 036001 (9
    pp.). [DOI: 10.1103/PhysRevMaterials.2.036001] "];
Print[" ----------------------------------------------------"];

NoL1 = 1; NoL2 = 2;
NoLp = NoL1;
Print[" I.0 The Units (nm, meV, AA)"];
"nm=10^(-9)m;";
nm = 10^(-9) m;
AA = 10^(-10) m;
JJkgms = kg m^2 / s^2;
Cl = Amper s;
"eV=JJ Electronp;";
JJ = eV / Electron;
JJms = (kg m^2) / s^2;
meV = N[eV / 1000];
Print["-------------------------------------------------------------"];

Print[" I.1. All Input Parameters and Constants--------------"];
Print[" I.1.1. The sampling parameters"]
npRIn1 = 1000;
Print["npRIn1=", npRIn1];
Print[" I.1.2. The Input Geometry Parameters of the system"];
L14d839nm = 14.839 nm;
L12d709nm = 12.709 nm;
L129d678nm = 29.678 nm;
L1p = L129d678nm;
L1p = L14d839nm;

Print[" The carbon nanoribbon length L1=", L1p / nm, "nm"];
Lw11d8nm = 11.8 nm;
Lwp = Lw11d8nm;
Print[" The carbon nanoribbon width Lw=", Lwp / nm, "nm"];
Print["  ---------------------------------------------  "];

Print[" Number of the layers in carbon nanoscroll NoL=", NoLp];
Print[" The length of a carbon nanoribbon L1=", L1p / nm, "nm"];
Lw1nm = 1. nm; Lwp = Lw1nm;
Print[" The carbon nanoribbon width Lw=", Lwp / nm, "nm"];
RIn1d1nm = 1.1 nm;
RIn1d2nm = 1.2 nm;
RIn1d14nm = 1.14 nm;
RIn2nm = 2.047 nm;
RIn2d1nm = 2.1 nm;
RIn2d2nm = 2.2 nm;
RIn2d3nm = 2.3 nm;
RIn2d4nm = 2.4 nm;
RIn2d5nm = 2.5 nm;
RIn2d6nm = 2.6 nm;
RIn1p = RIn2d5nm;
RIn1p = RIn2d3nm;
RIn1p = RIn2d2nm;
```

```
RIn1p = RIn2d1nm;
RIn1p = RIn1d14nm;
Print[" The inner radius of the nanoscroll RIn1=", RIn1p / nm, "nm"];
Print[" I.1.2. The Input Energy Constants"];
Print[" epsVdW - the interlayer interaction energy per one atom of"];
Print[" the nanoscroll:"];
epsVdW35 = 35.0 meV / atom; epsVdWp = epsVdW35;
Print[" epsVdW=", epsVdWp / (eV / atom), "eV/atom"];
Print[" C - the bending elastic constant:"];
C201 = 2.01 eV AA ^ 2 / atom;
CBN1328 = 1.328 eV AA ^ 2 / atom;
CCp = C201;
CBNp = CBN1328;
CBNp = CCp;
Print[" CCelast=", CCp / (eV AA ^ 2 / atom), "eV AA^2/atom"];
Print[" CCBNelast=", CBNp / (eV AA ^ 2 / atom), "eV AA^2/atom"];
Print[" I.1.3.The Input Geometry constants--------------"];
Print[" The interatomic distance aCC and the interlayer distance h"];
aCC142AA = 1.42 AA; aCCp = aCC142AA;
h335nm = 0.3354 nm; hp = h335nm;
Print["h=", hp / nm, " nm  (Interlayer distance)"];
Print[" aCC=", aCCp / nm, "nm, h=", hp / nm, "nm"];
NatomsInCell2 = 2; NatomsInCellp = NatomsInCell2;
Print["NatomsInCell=", NatomsInCellp];

Print[" dPhi12 - The difference of the inner angles of the spirales"];
Print["   of the Layers"];
dPhi12eq0 = 0.0 Pi;
dPhi12eqPi = 1.0 Pi;
dPhi12p = 0.0 Pi;
dPhi12p = 1.0 Pi;
dPhi12p = 0.5 Pi;
Print[" I.5.The parameters for the visualisation"];
RIn1MinMonoScroll = hp / 5;
RIn1MinBiScroll = hp / 5;
RIn1MaxMonoScroll = 4 nm;
RIn1MaxBiScroll = 8 nm;
PlotRangeMonoScroll = {-4 eV / atom, 12 eV / atom};
PlotRangeBiScroll = {-10 eV / atom, 30 eV / atom};
ShowSpirales = True;
ShowThePlot = True;
Print[" I.6. The parameters of the output file"];
NanoscrollNamep = StringJoin["Nanoscroll", ToString[NoLp], "L", ToString[L1p / nm], "nm"];
Print[" NanoscrollName=", NanoscrollNamep];
CarbonNanoscrollEnergyVsRInFileName = StringJoin[NanoscrollNamep, ".txt"];
Print[CarbonNanoscrollEnergyVsRInFileName];
Print[" (The output of the data to a file Is Not Performed)"];
npRIn1 = 1000;
Print[" The number of the output points = ", npRIn1];
Print[" I.7. The Input Numerical Constants used in the programm"];
Print[" The Indexes used for the work with EVdW[...] function"];
iEVdW = 1; iEVdW1Un1 = 2; iEVdW1Ov1 = 3; iEVdW1Un2 = 4; iEVdW1Ov2 = 5;
iEVdW2Un1 = 6; iEVdW2Ov1 = 7;
Print[" --------End of the Input---------------"];
AA = 0.1 nm; PhiIn := φIn; PhiOut := φOut;
Print["-------------------------------------------------------------"];
```

```
Print[" II. The derivated parameters and the functions required"];
Print[" II.1. The derivated parameters"];
fSa[aCC_] := aCC^2 3 Sqrt[3] / 4; fSa[aCCp]; Sap = fSa[aCCp];
Print["  The cell area Sa=", fSa[aCC], "=", Sap / nm^2, "nm^2"];
Print[" II.2. The required functions--------------"];
Print[" II.2.1. The function fSpiraleLen[", NoLp, ",φIn, φOut, h] defines"];
Print[
  "  the Length of a Spirale with the inner agle φIn and the outer angle φOut(>=φIn):"];
fSpiraleLen[NoLv_, PhiInv_, PhiOutv_, hv_] :=
 (1 / (4 Pi) hv NoLv (-PhiInv Sqrt[1 + PhiInv^2] +
    PhiOutv Sqrt[1 + PhiOutv^2] - ArcSinh[PhiInv] +
    ArcSinh[PhiOutv]));
Print["  fSpiraleLen[", NoLp,
  ", φIn, φOut, h]=", fSpiraleLen[NoLp, PhiIn, PhiOut, h], "."];
Print[" II.2.2. The function fElast[φIn,ρOut] is
    required to calculate an nanoscrollelastic energy: "];
fElast[PhiInv_,
  PhiOutv_] := (Sqrt[PhiInv^2 + 1] / PhiInv -
  Sqrt[PhiOutv^2 + 1] / PhiOutv - ArcSinh[PhiInv] + ArcSinh[PhiOutv]);
Print[" fElast[φIn,φOut] = ", fElast[PhiIn, PhiOut], "."];
Print[" II.2.3. Define the function fPhiOutvsPhiInLh[", NoLp, ",", PhiIn, ",L,h]."]
fPhiOutvsPhiInLh[NoLv_, PhiInv_, Lv_, hv_] :=
 Sqrt[4 π Lv / (NoLv hv) + PhiInv^2];
Print[" The function fPhiOutvsPhiInLh[", NoLp,
  ",", PhiIn, ",L,h]=", fPhiOutvsPhiInLh[NoLp, PhiIn, L, h], " is a
 good approximation to obtain the value of φOut for the defined φIn,L,h."];
fPhiInvsPhiOutLh[NoLv_, PhiOutv_, Lv_, hv_] :=
 Sqrt[PhiOutv^2 - 4 π Lv / (NoLv hv)];
Print[" The inverse function fPhiInvsPhiOutLh[", NoLp, ",φOut, L, h]]=",
 fPhiInvsPhiOutLh[NoLp, PhiOut, L, h]];
Print[" could be used in the program applications
    if ROut (instead of RIn) is the input parameter of the system."];

Print[" II.2.4. The functions
    fSpirale1Under(Over)Spirale1Length[NoLv,PhiIn1v ,PhiOut1v,hv]" ];
fSpirale1UnderSpirale1Length[NoLv_, PhiIn1v_ , PhiOut1v_, hv_] :=
  fSpiraleLen[NoLv, PhiIn1v , PhiOut1v - 2 Pi, hv];
fSpirale1OverSpirale1Length[NoLv_, PhiIn1v_ , PhiOut1v_, hv_] :=
  fSpiraleLen[NoLv, PhiIn1v + 2 Pi , PhiOut1v, hv];

fSpirale1UnderSpirale2Length[NoLv_, PhiIn1v_ , PhiOut1v_, hv_, dPhi12v_] :=
  fSpiraleLen[NoLv, PhiIn1v, PhiOut1v - 2 Pi / NoLv, hv];
fSpirale1OverSpirale2Length[NoLv_, PhiIn1v_ , PhiOut1v_, hv_, dPhi12v_] :=
  fSpiraleLen[NoLv, PhiIn1v + 2 Pi / NoLv + dPhi12v, PhiOut1v, hv];
fSpirale2UnderSpirale1Length[NoLv_, PhiIn1v_ , PhiOut1v_, hv_, dPhi12v_] :=
  fSpiraleLen[NoLv, PhiIn1v, PhiOut1v - 2 Pi / NoLv, hv];
fSpirale2OverSpirale1Length[NoLv_, PhiIn1v_ , PhiOut1v_, hv_, dPhi12v_] :=
  fSpiraleLen[NoLv, PhiIn1v - dPhi12v + 2 Pi / NoLv, PhiOut1v - dPhi12v, hv];

Print["  These functiona are not required, dut could be helpful),"];

If[NoLp == 1,
Print["fSpirale1UnderSpirale1Length[1,PhiIn1v ,PhiOut1v,hv]="];
Print["  =fSpiraleLen[NoLv,PhiIn1v ,PhiOut1v-2Pi,hv]=",
   fSpiraleLen[NoLv, PhiIn1v , PhiOut1v - 2 Pi, hv], ";"];
Print["  fSpirale1UnderSpirale1Length[NoLp,PhiIn1p
     ,PhiOut1p,hp]=fSpirale1UnderSpirale1Length[", NoLp, ",",
```

```
   PhiIn1p / (2 Pi), "(2Pi),", PhiOut1p / (2 Pi), "(2Pi),", hp / nm, "nm] ="];
Print["  =", fSpirale1UnderSpirale1Length[NoLp, PhiIn1p , PhiOut1p, hp] / nm, "nm."];

Print["fSpirale1OverSpirale1Length[1,PhiIn1v ,PhiOut1v,hv]="];
Print["  =fSpiraleLen[NoLv,PhiIn1v+2Pi ,PhiOut1v,hv]=",
   fSpiraleLen[NoLv, PhiIn1v + 2 Pi , PhiOut1v, hv], ";"];
Print["  fSpirale1OverSpirale1Length[NoLp,PhiIn1p
     ,PhiOut1p,hp]=fSpirale1OverSpirale1Length[", NoLp, ",",
   PhiIn1p / (2 Pi), "(2Pi),", PhiOut1p / (2 Pi), "(2Pi),", hp / nm, "nm] ="];
Print["  =", fSpirale1OverSpirale1Length[NoLp, PhiIn1p , PhiOut1p, hp] / nm, "nm."];
];

If[NoLp == 2,
Print["  fSpirale1UnderSpirale2Length[1,PhiIn1v ,PhiOut1v,hv,dPhi12v]="];
Print["  fSpiraleLen[NoLv,PhiIn1v, PhiOut1v -2 Pi/NoLv,hv]=",
   fSpirale1UnderSpirale2Length[1, PhiIn1v , PhiOut1v, hv, dPhi12v], ";"];
Print["fSpirale1UnderSpirale2Length[NoLp,PhiIn1p
     ,PhiOut1p,hp,dPhi12p]=fSpirale1UnderSpirale2Length[",
   NoLp, ",", PhiIn1p / (2 Pi), "(2Pi),", PhiOut1p / (2 Pi), "(2Pi),", hp / nm,
   "nm,", dPhi12p / (2 Pi), "(2Pi)] ="];
Print["  =", fSpirale1UnderSpirale2Length[NoLp, PhiIn1p , PhiOut1p, hp, dPhi12p] / nm,
   "nm."];
Print["  fSpirale1OverSpirale2Length[1,PhiIn1v ,PhiOut1v,hv,dPhi12v]="];
Print["  =fSpiraleLen[NoLv,PhiIn1v+Pi ,PhiOut1v,hv]=",
   fSpiraleLen[NoLv, PhiIn1v + Pi , PhiOut1v, hv], ";"];
Print["fSpirale1OverSpirale2Length[NoLp,PhiIn1p
     ,PhiOut1p,hp]=fSpirale1OverSpirale1Length[", NoLp, ",",
   PhiIn1p / (2 Pi), "(2Pi),", PhiOut1p / (2 Pi), "(2Pi),", hp / nm, "nm] ="];
Print["  =", fSpirale1OverSpirale2Length[NoLp, PhiIn1p , PhiOut1p, hp, dPhi12p] / nm,
   "nm."];
Print[""];
Print["  fSpirale2UnderSpirale1Length[1,PhiIn1v ,PhiOut1v,hv]="];
Print["  fSpiraleLen[NoLv,PhiIn1v, PhiOut1v -2 Pi/NoLv,hv]=",
   fSpirale1UnderSpirale2Length[1, PhiIn1v , PhiOut1v, hv, dPhi12v], ";"];
Print["fSpirale2UnderSpirale1Length[NoLp,PhiIn1p
     ,PhiOut1p,hp,dPhi12p]=fSpirale2UnderSpirale1Length[",
   NoLp, ",", PhiIn1p / (2 Pi), "(2Pi),", PhiOut1p / (2 Pi), "(2Pi),", hp / nm,
   "nm,", dPhi12p / (2 Pi), "(2Pi)] ="];
Print["  =", fSpirale1UnderSpirale2Length[NoLp, PhiIn1p , PhiOut1p, hp, dPhi12p] / nm,
   "nm."];
Print["  fSpirale1OverSpirale2Length[1,PhiIn1v ,PhiOut1v,hv]="];
Print["  =fSpiraleLen[NoLv,PhiIn1v+Pi ,PhiOut1v,hv]=",
   fSpiraleLen[NoLv, PhiIn1v + Pi , PhiOut1v, hv], ";"];
Print["fSpirale1OverSpirale2Length[NoLp,PhiIn1p
     ,PhiOut1p,hp]=fSpirale1OverSpirale2Length[", NoLp, ",",
   PhiIn1p / (2 Pi), "(2Pi),", PhiOut1p / (2 Pi), "(2Pi),", hp / nm, "nm] ="];
Print["  =", fSpirale1OverSpirale2Length[NoLp, PhiIn1p , PhiOut1p, hp, dPhi12p] / nm,
   "nm."];
];

Print[" II.2.4. The function fRIn1Sharp[NoLv,L1v,hv]"]
fRIn1Sharp[NoLv_, L1v_, hv_] := (L1v / (2 Pi) - (NoLv hv / 2));
Print["fRIn1Sharp[NoLv,L1v,hv]=", fRIn1Sharp[NoLv, L1v, hv]];
Print["is a good approximation to obtain
    the value of the sharp in the dependence ScrollEnergy[RIn]"];
Print["fRIn1Sharp[", NoLp, ", ", L1p / nm, "nm, ", hp / nm, "nm] = ",
  fRIn1Sharp[NoLp, L1p, hp] / nm, "nm"];
```

```
Print["------------------------------------------------------------"];

Print[" III. Begin of Calculation "];
If[NoLp == 1,
Print[" III.1. The inner and the outer angle of the spirale of the layer:"]];
If[NoLp == 2,
Print[" III.1. The inner and the outer angles of the spirales of the layers:"]];
Print[" φIn1=", RIn1 2 Pi / (NoLp h) , ", φOut1=fPhiOutvsPhiInLh[", NoLp, ",ϕIn1,L1,h];"];
fPhiIn1[NoLv_, RIn1v_, hv_] := RIn1v 2 Pi / (NoLv hv);
PhiIn1p = fPhiIn1[NoLp, RIn1p, hp];
fPhiOut1[NoLv_, L1v_, RIn1v_, hv_] :=
 fPhiOutvsPhiInLh[NoLv, fPhiIn1[NoLv, RIn1v, hv], L1v, hv];
Print[" For RIn1=", RIn1p / nm, "nm,h=", hp / nm, "nm:"];
PhiOut1p = fPhiOut1[NoLp, L1p, RIn1p, hp];
ROut1p = PhiOut1p NoLp hp / (2 Pi);
Print[" φIn1=", PhiIn1p / (2 Pi), "(2Pi),ΨOut1=", PhiOut1p / (2 Pi), "(2Pi)."];
fPhiIn2[NoLv_, RIn1v_, hv_, dPhi12v_] :=
 fPhiIn1[NoLv, RIn1v, hv] + dPhi12v;
PhiIn2dPhi12p =
 fPhiIn2[NoLp, RIn1p, hp, 0]; (*www orig 2022.10*)
PhiIn2dPhi12p =
 fPhiIn2[NoLp, RIn1p, hp, dPhi12p]; (* for dPhi12p!=0, checked 2022.10*)
PhiIn2dPhi12Pip =
 fPhiIn2[NoLp, RIn1p, hp, Pi];
fPhiOut2[NoLv_, L1v_, RIn1v_, hv_, dPhi12v_] :=
 fPhiOutvsPhiInLh[NoLv, fPhiIn2[NoLv, RIn1v, hv, dPhi12v], L1v, hv];
PhiOut2dPhi12p =
 fPhiOut2[NoLp, L1p, RIn1p, hp, dPhi12p];
If[NoLp == 2, Print["  φIn2=", PhiIn2dPhi12p / (2 Pi),
   "(2Pi),φOut2=", PhiOut2dPhi12p / (2 Pi), "(2Pi)"];
PhiOut2dPhi12Pip =
 fPhiOut2[NoLp, L1p, RIn1p, hp, Pi];
Print[" for dφ12=Pi: PhiIn2=", PhiIn2dPhi12Pip / (2 Pi),
   "(2Pi),φOut2=", PhiOut2dPhi12Pip / (2 Pi), "(2Pi)"];];
Print["L1=", L1p / nm, "nm, RIn1=", RIn1p / nm, "nm"];
If[NoLp == 1, Print[" Plot the Spirale of the layer:"]];
If[NoLp == 2, Print[" Plot Spirales of the layers:"]]; "for dφ12=0";
Spirale1Plot =
 PolarPlot[(Phiv) NoLp hp / (2 Pi) / nm, {Phiv, PhiIn1p,
  PhiOut1p},
  PlotRange -> {{-1.1 ROut1p / nm, 1.1 ROut1p / nm}, {-1.1 ROut1p / nm,
   1.1 ROut1p / nm}}, PlotStyle -> {Red, Thin}, Axes -> None];
If[NoLp == 1, Print[Show[Spirale1Plot]];];
If[NoLp > 1,
Print[" Plot the Spirale of the layers:"];
Spirale2Plot = PolarPlot[(Phiv - Pi) NoLp hp / (2 Pi) / nm,
   {Phiv, PhiIn2dPhi12p + Pi, PhiOut2dPhi12p + Pi},
  PlotRange -> {{-1.1 ROut1p / nm, 1.1 ROut1p / nm}, {-1.1 ROut1p / nm,
   1.1 ROut1p / nm}}, PlotStyle -> {Blue, Thin}, Axes -> None];
Spirale2dPhi12PiPlot = PolarPlot[(Phiv - Pi) NoLp hp / (2 Pi) / nm,
   {Phiv, PhiIn2dPhi12p + Pi, PhiOut2dPhi12Pip + Pi},
  PlotRange -> {{-1.1 ROut1p / nm, 1.1 ROut1p / nm}, {-1.1 ROut1p / nm,
   1.1 ROut1p / nm}}, PlotStyle -> {Blue, Thin}, Axes -> None];
Print[Show[{Spirale1Plot, Spirale2Plot}]];
]
If[NoLp == 1,
 Spirale1OverSpirale1Plot =
```

```
  If[PhiIn1p + 2 Pi < PhiOut1p,
   PolarPlot[(Phiv) NoLp hp / (2 Pi) /nm, {Phiv, PhiIn1p + 2 Pi,
    PhiOut1p},
    PlotRange -> {{-1.1 ROut1p /nm, 1.1 ROut1p /nm}, {-1.1 ROut1p /nm,
      1.1 ROut1p /nm}}, PlotStyle -> {Red, Thick}, Axes -> None], {}];
 Spirale1UnderSpirale1Plot =
  If[PhiIn1p < PhiOut1p - 2 Pi,
   PolarPlot[(Phiv) NoLp hp / (2 Pi) /nm, {Phiv, PhiIn1p,
    PhiOut1p - 2 Pi},
    PlotRange -> {{-1.1 ROut1p /nm, 1.1 ROut1p /nm}, {-1.1 ROut1p /nm,
      1.1 ROut1p /nm}}, PlotStyle -> {Red, Thick}, Axes -> None], {}];
 Print[" {Spirale,Spirale1UnderSpirale1},{Spirale1,Spirale1OverSpirale1}:"];
 Print[Show[{Spirale1Plot, Spirale1UnderSpirale1Plot}],
  Show[{Spirale1Plot, Spirale1OverSpirale1Plot}]];
];
If[NoLp == 2,
Spirale1UnderSpirale2dPhi120Plot =
  If[PhiIn1p < PhiOut2dPhi12p - Pi,
   PolarPlot[(Phiv) NoLp hp / (2 Pi) /nm, {Phiv, PhiIn1p,
    PhiOut2dPhi12p - Pi}, PlotStyle -> {Red, Thick},
    PlotRange -> {{-1.1 ROut1p /nm, 1.1 ROut1p /nm}, {-1.1 ROut1p /nm,
      1.1 ROut1p /nm}}], {}];
Spirale1OverSpirale2dPhi120Plot =
  If[PhiIn1p + Pi < PhiOut1p,
   PolarPlot[(Phiv) NoLp hp / (2 Pi) /nm, {Phiv,
    PhiIn1p + Pi +
     dPhi12p, PhiOut1p},
    PlotStyle -> {Red, Thick},
    PlotRange -> {{-1.1 ROut1p /nm, 1.1 ROut1p /nm}, {-1.1 ROut1p /nm,
      1.1 ROut1p /nm}}], {}];
Spirale2UnderSpirale1dPhi120Plot =
  If[PhiIn2dPhi12p + Pi < PhiOut1p,
   PolarPlot[(Phiv - Pi) NoLp hp / (2 Pi) /nm, {Phiv,
    PhiIn2dPhi12p + Pi, PhiOut1p}, PlotStyle -> {Blue, Thick},
    PlotRange -> {{-1.1 ROut1p /nm, 1.1 ROut1p /nm}, {-1.1 ROut1p /nm,
      1.1 ROut1p /nm}}], {}];
Spirale2OverSpirale1dPhi120Plot =
  If[2 Pi + PhiIn2dPhi12p -
    dPhi12p <
    PhiOut2dPhi12p + Pi,
   PolarPlot[(Phiv - Pi) NoLp hp / (2 Pi) /nm, {Phiv,
    2 Pi + PhiIn2dPhi12p -
     dPhi12p,
    PhiOut2dPhi12p + Pi}, PlotStyle -> {Blue, Thick},
    PlotRange -> {{-1.1 ROut1p /nm, 1.1 ROut1p /nm}, {-1.1 ROut1p /nm,
      1.1 ROut1p /nm}}], {}];
Print[
   "Plot Spirales for dPhi12=Pi (could be NotRequired, dPhi12=0 in this program)"];
Spirale1UnderSpirale2dPhi12PiPlot =
  If[PhiIn1p < PhiOut2dPhi12Pip - Pi,
   PolarPlot[(Phiv) NoLp hp / (2 Pi) /nm, {Phiv, PhiIn1p,
    PhiOut2dPhi12Pip - Pi}, PlotStyle -> {Red, Thick},
    PlotRange -> {{-1.1 ROut1p /nm, 1.1 ROut1p /nm}, {-1.1 ROut1p /nm,
      1.1 ROut1p /nm}}], {}];
Spirale1OverSpirale2dPhi12PiPlot =
  If[PhiIn1p + Pi +
    dPhi12p < PhiOut1p,
```

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  PolarPlot[(Phiv) NoLp hp / (2 Pi) / nm, {Phiv,
   PhiIn1p + Pi +
    dPhi12p, PhiOut1p},
   PlotStyle -> {Red, Thick},
   PlotRange -> {{-1.1 ROut1p / nm, 1.1 ROut1p / nm}, {-1.1 ROut1p / nm,
     1.1 ROut1p / nm}}], {}];
Spirale2UnderSpirale1dPhi12PiPlot =
 If[PhiIn2dPhi12p + Pi < PhiOut1p,
  PolarPlot[(Phiv - Pi) NoLp hp / (2 Pi) / nm, {Phiv,
   PhiIn2dPhi12Pip + Pi, PhiOut1p}, PlotStyle -> {Blue, Thick},
   PlotRange -> {{-1.1 ROut1p / nm, 1.1 ROut1p / nm}, {-1.1 ROut1p / nm,
     1.1 ROut1p / nm}}], {}];
Spirale2OverSpirale1dPhi12PiPlot =
 If[2 Pi + PhiIn2dPhi12Pip -
   dPhi12p <
   PhiOut2dPhi12Pip + Pi,
  PolarPlot[(Phiv - Pi) NoLp hp / (2 Pi) / nm, {Phiv,
   2 Pi + PhiIn2dPhi12Pip -
    dPhi12p,
   PhiOut2dPhi12Pip + Pi}, PlotStyle -> {Blue, Thick},
   PlotRange -> {{-1.1 ROut1p / nm, 1.1 ROut1p / nm}, {-1.1 ROut1p / nm,
     1.1 ROut1p / nm}}], {}];

 Print[" {Spirale1,Spirale2,Spirale1UnderSpirale2,Spirale2UnderSpirale1},"];
 Print["     {Spirale1,Spirale2,Spirale1OverSpirale2,Spirale2OverSpirale1}"];
 Print[" for dPhi12=0: ", Show[Spirale1Plot, Spirale2Plot],
  Show[Spirale1Plot, Spirale2Plot, Spirale1UnderSpirale2dPhi120Plot,
   Spirale2UnderSpirale1dPhi120Plot],
  Show[Spirale1Plot, Spirale2Plot, Spirale1OverSpirale2dPhi120Plot,
   Spirale2OverSpirale1dPhi120Plot]];
 Print[" for dPhi12=Pi: ", Show[Spirale1Plot, Spirale2dPhi12PiPlot],
  Show[Spirale1Plot, Spirale2dPhi12PiPlot, Spirale1UnderSpirale2dPhi12PiPlot,
   Spirale2UnderSpirale1dPhi12PiPlot],
  Show[Spirale1Plot, Spirale2dPhi12PiPlot, Spirale1OverSpirale2dPhi12PiPlot,
   Spirale2OverSpirale1dPhi12PiPlot]];

];

Print[" III.2. The nanoscroll energy calculation"];
Print[" III.2.1. The elastic energy calculation"];
fEelastCC[NoLv_, Lwv_, L1v_, RIn1v_, hv_, aCCv_, CCv_] :=
 Module[{},
  Return[2 Pi CCv Lwv / (hv fSa[aCCv]) fElast[
    fPhiIn1[NoLv, RIn1v, hv],
    fPhiOut1[NoLv, L1v, RIn1v, hv]]];];
fEelastCBN[NoLv_, Lwv_, L1v_, RIn1v_, hv_, aCCv_, CBNv_] :=
 Module[{},
  Return[2 Pi CBNv Lwv / (hv fSa[aCCv]) fElast[
    fPhiIn1[NoLv, RIn1v, hv],
    fPhiOut1[NoLv, L1v, RIn1v, hv]]];];
EelastCCp = fEelastCC[NoLp, Lwp, L1p, RIn1p, hp, aCCp, CCp];
EelastCBNp = fEelastCBN[NoLp, Lwp, L1p, RIn1p, hp, aCCp, CBNp];
Print[" EelastC=", EelastCCp / (eV / atom), "eV/atom"];
If[NoLp == 2, Print[" EelastBN=", EelastCBNp / (eV / atom), "eV/atom"];];
Print[" III.2.2. The Van-der-Waals energy calculation"];
"The definition of the function ";
"'fEVdWLayer1Overlap[NoLv,Lwv,L1v, RIn1v, hv, aCCv, epsVdWv]'";
```

```
"(Note: This function is omitted at calculations";
"    but could be helpful at
   calculation of VdW ebergy of monoscroll at debugging;";
"    for example,";
"    fEVdWLayer1Overlap[NoL1,Lwp,15nm, 2nm, hp, aCCp, epsVdWp] ";
" and fEVdWLayersOverlap[NoL2,Lwp,L1p=15nm, 2nm, hp, aCCp, epsVdWp, 0]";
"    give the same values";
fEVdWLayer1Overlap[NoLv_, Lwv_, L1v_, RIn1v_, hv_, aCCv_, epsVdWv_] := Module[
{EVdWv,
 EVdW1Un1v = 0 (eV / atom), EVdW1Ov1v = 0 (eV / atom),
 Spirale1UnderSpirale1Length = 0 nm, Spirale1OverSpirale1Length = 0 nm,
 PhiIn1v = fPhiIn1[NoLv, RIn1v, hv],
 PhiOut1v = fPhiOut1[NoLv, L1v, RIn1v, hv],
 },
Spirale1OverSpirale1Length = fSpiraleLen[NoLv, PhiIn1v + 2 Pi, PhiOut1v, hv];
Spirale1UnderSpirale1Length = fSpiraleLen[NoLv, PhiIn1v , PhiOut1v - 2 Pi, hv];
"Note: Spirale1OverSpirale1Length>Spirale1UnderSpirale1Length";
EVdW1Un1v = -epsVdWv Lwv / (2 fSa[aCCv]) Spirale1UnderSpirale1Length;
EVdW1Ov1v = -epsVdWv Lwv / (2 fSa[aCCv]) Spirale1OverSpirale1Length;
EVdWv = (EVdW1Un1v + EVdW1Ov1v);
Return[{EVdWv, EVdW1Un1v, EVdW1Ov1v}];
];
"The definition of the function";
"fEVdWLayersOverlap[NoLv_,Lwv_,L1v_, RIn1v_, hv_, aCCv_, epsVdWv_, dPhi12v_]";
fEVdWLayersOverlap[NoLv_, Lwv_, L1v_, RIn1v_, hv_, aCCv_, epsVdWv_, dPhi12v_] := Module[
{EVdW,
 EVdW1Un1 = 0 (eV / atom), EVdW1Ov1 = 0 (eV / atom),
 EVdW1Un2 = 0 (eV / atom), EVdW1Ov2 = 0 (eV / atom),
 EVdW2Un1 = 0 (eV / atom), EVdW2Ov1 = 0 (eV / atom),
 Spirale1UnderSpirale1Length = 0 nm, Spirale1OverSpirale1Length = 0 nm,
 Spirale1UnderSpirale2Length = 0 nm, Spirale1OverSpirale2Length = 0 nm,
 Spirale2UnderSpirale1Length = 0 nm, Spirale2OverSpirale1Length = 0 nm,
 PhiIn1 = fPhiIn1[NoLv, RIn1v, hv],
 PhiIn2 = fPhiIn2[NoLv, RIn1v, hv, dPhi12v],
 PhiOut1 = fPhiOut1[NoLv, L1v, RIn1v, hv],
 PhiOut2 = fPhiOut2[NoLv, L1v, RIn1v, hv, dPhi12v],
 ReturnEnergiesv = {1, 2, 3, 4, 5, 6, 7}
},
If[NoLv == 1,
If[PhiIn1 < PhiOut1 - 2 Pi,
     Spirale1UnderSpirale1Length = fSpiraleLen[NoLv, PhiIn1, PhiOut1 - 2 Pi, hv];];
If[PhiIn1 + 2 Pi < PhiOut1, Spirale1OverSpirale1Length =
       fSpiraleLen[NoLv, PhiIn1 + 2 Pi, PhiOut1, hv];];
EVdW1Un1 = -epsVdWv Lwv / (2 fSa[aCCv]) Spirale1UnderSpirale1Length;
EVdW1Ov1 = -epsVdWv Lwv / (2 fSa[aCCv]) Spirale1OverSpirale1Length;
EVdW = (EVdW1Un1 + EVdW1Ov1);
ReturnEnergiesv = {EVdW, EVdW1Un1, EVdW1Ov1};
];
If[NoLv == 2,
  If[PhiIn1 < PhiOut2 - Pi,
     Spirale1UnderSpirale2Length = fSpiraleLen[NoLv, PhiIn1, PhiOut2 - Pi, hv];];
  If[PhiIn1 + Pi + dPhi12v < PhiOut1, Spirale1OverSpirale2Length =
       fSpiraleLen[NoLv, PhiIn1 + Pi + dPhi12v, PhiOut1, hv];];
  If[PhiIn1 + dPhi12v < PhiOut1 - Pi, Spirale2UnderSpirale1Length =
       fSpiraleLen[NoLv, PhiIn1 + dPhi12v, PhiOut1 - Pi, hv];];
  If[PhiIn1 - dPhi12v + Pi < PhiOut2 - dPhi12v, Spirale2OverSpirale1Length =
       fSpiraleLen[NoLv, PhiIn1 - dPhi12v + Pi, PhiOut2 - dPhi12v, hv];];
```

```
EVdW1Un2 = -epsVdWv Lwv / (2 fSa[aCCv]) Spirale1UnderSpirale2Length;
  EVdW1Ov2 = -epsVdWv Lwv / (2 fSa[aCCv]) Spirale1OverSpirale2Length;
  EVdW2Un1 = -epsVdWv Lwv / (2 fSa[aCCv]) Spirale2UnderSpirale1Length;
  EVdW2Ov1 = -epsVdWv Lwv / (2 fSa[aCCv]) Spirale2OverSpirale1Length;
  EVdW = (EVdW1Un2 + EVdW1Ov2 + EVdW2Un1 + EVdW2Ov1);
  ReturnEnergiesv[[iEVdW]] = EVdW;
  ReturnEnergiesv[[iEVdW1Un2]] = EVdW1Un2;
  ReturnEnergiesv[[iEVdW1Ov2]] = EVdW1Ov2;
  ReturnEnergiesv[[iEVdW2Un1]] = EVdW2Un1;
  ReturnEnergiesv[[iEVdW2Ov1]] = EVdW2Ov1;
];
Return[ReturnEnergiesv];
];

EVdWdPhi12eq0allp =
 fEVdWLayersOverlap[NoL2, Lwp, L1p, RIn1p, hp, aCCp, epsVdWp, dPhi12eq0];
EVdWvardPhi12allp =
 fEVdWLayersOverlap[NoLp, Lwp, L1p, RIn1p, hp, aCCp, epsVdWp, dPhi12p];
If[NoLp == 1,
Print[" EVdWvardPhi12allp[[iEVdW]]=",
   EVdWvardPhi12allp[[iEVdW]] / (eV / atom), "eV/atom"];
Print["( EVdWvardPhi12allp[[iEVdW1Un1]]=",
   EVdWvardPhi12allp[[iEVdW1Un1]] / (eV / atom), "eV/atom"];
 Print["  EVdWvardPhi12allp[[iEVdW1Ov1]]=",
   EVdWvardPhi12allp[[iEVdW1Ov1]] / (eV / atom), "eV/atom  )"];
];
If[NoLp == 2,
Print[" for dPhi12=", dPhi12p / Pi, "Pi EVdWvardPhi12allp[[iEVdW]]=",
 EVdWvardPhi12allp[[iEVdW]] / (eV / atom), "eV/atom"];
 Print[" For dPhi12=", dPhi12eq0 / Pi, "Pi:"];
 Print[" EVdWvardPhi12allp[[iEVdW]]=",
 EVdWdPhi12eq0allp[[iEVdW]] / (eV / atom), "eV/atom"];
 Print[" EVdWvardPhi12allp[[iEVdW1Un2]]=",
 EVdWdPhi12eq0allp[[iEVdW1Un2]] / (eV / atom), "eV/atom"];
 Print[" EVdWvardPhi12allp[[iEVdW1Ov2]]=",
 EVdWdPhi12eq0allp[[iEVdW1Ov2]] / (eV / atom), "eV/atom"];
 Print[" EVdWvardPhi12allp[[iEVdW2Un1]]=",
 EVdWdPhi12eq0allp[[iEVdW2Un1]] / (eV / atom), "eV/atom"];
 Print[" EVdWvardPhi12allp[[iEVdW2Ov2]]=",
 EVdWdPhi12eq0allp[[iEVdW2Ov1]] / (eV / atom), "eV/atom"];
 EVdWdPhi12eqPiallp =
 fEVdWLayersOverlap[NoLp, Lwp, L1p, RIn1p, hp, aCCp, epsVdWp, dPhi12eqPi];
(**) Print[" For dPhi12=", dPhi12eqPi / Pi, "Pi:"];
 Print[" EVdWvatdPhi12allp[[iEVdW]]=",
 EVdWdPhi12eqPiallp[[iEVdW]] / (eV / atom), "eV/atom"];
 Print[" EVdWvatdPhi12allp[[iEVdW1Un2]]=",
 EVdWdPhi12eqPiallp[[iEVdW1Un2]] / (eV / atom), "eV/atom"];
 Print[" EVdWvatdPhi12allp[[iEVdW1Ov2]]=",
 EVdWdPhi12eqPiallp[[iEVdW1Ov2]] / (eV / atom), "eV/atom"];
 Print[" EVdWvatdPhi12allp[[iEVdW2Un1]]=",
 EVdWdPhi12eqPiallp[[iEVdW2Un1]] / (eV / atom), "eV/atom"];
 Print[" EVdWvatdPhi12allp[[iEVdW2Ov2]]=",
 EVdWdPhi12eqPiallp[[iEVdW2Ov1]] / (eV / atom), "eV/atom"];
 EVdWEVdWdPhi12eq0p = EVdWdPhi12eq0allp[[iEVdW]];
 Print[" EVdWdPhi12eq0allp=", EVdWdPhi12eq0allp / (eV / atom),
 "eV/atom"];
 EVdWEVdWdPhi12eqPip = EVdWvardPhi12allp[[iEVdW]];
```

```
 Print[" EVdWEVdWdPhi12eqPip=", EVdWEVdWdPhi12eqPip / (eV / atom),
  "eV/atom"];
(**)
];
If[NoLp == 2, Print[" III.3. The energy of flat planes "];];
fEnergyFlatPlanes[NoLv_, Lwv_, L1v_, aCCv_, epsVdWv_] :=
  If[NoLv == 2, -epsVdWv Lwv / fSa[aCCv] L1v, 0 eV / atom];
EnergyFlatPlanesp = fEnergyFlatPlanes[NoLp, Lwp, L1p, aCCp, epsVdWp];
If[NoLp == 2, Print[" EnergyFlatPlanes=-eps width/Sa L1(NoL-1) =",
 EnergyFlatPlanesp / (eV / atom), "eV/atom"];];
Print[" III.4. The total energy of the nanoscroll"];
fScrollEnergydPhi[NoLv_, Lwv_, L1v_,
   RIn1v_, hv_, aCCv_, epsVdWv_, CCv_, CBNv_, dPhi12v_] :=
 Module[{ScrollEnergyv, EVdWv, EVdWnoDimv},
 EVdWv = fEVdWLayersOverlap[NoLv, Lwv, L1v, RIn1v, hv, aCCv, epsVdWv, dPhi12v][[1]];
EVdWnoDimv = EVdWv /. {eV -> 1, atom -> 1, nm -> 1};
 If[NoLv == 1,
   If[EVdWnoDimv == 0, ScrollEnergyv = fEelastCC[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CCv],
    ScrollEnergyv = EVdWv + fEelastCC[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CCv];];
  ];
 If[NoLv == 2,
If[EVdWnoDimv == 0,
    ScrollEnergyv = fEelastCC[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CCv] +
    fEelastCBN[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CCv],
    ScrollEnergyv = EVdWv + fEelastCC[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CCv] +
    fEelastCBN[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CCv];];
 ];
 Return[ScrollEnergyv];
];

fScrollEnergyVdWandElast[NoLv_, Lwv_,
   L1v_, RIn1v_, hv_, aCCv_, epsVdWv_, CCv_, CBNv_] :=
 Module[{ ScrollEnergyVdWandElastv, EVdWv},
(*If[NoLv == 1,
 EVdWv=fEVdWLayer1Overlap[NoLv,Lwv,L1v,RIn1v,hv,aCCv,epsVdWv][[1]];
];
If[NoLv == 2,
 EVdWv=fEVdWLayersOverlap[NoLv,Lwv,L1v,RIn1v,hv,aCCv,epsVdWv][[1]];
];*)
EVdWv = fEVdWLayer1Overlap[NoLv, Lwv, L1v, RIn1v, hv, aCCv, epsVdWv][[1]];
If[NoLv == 1,
 ScrollEnergyVdWandElastv = EVdWv + fEelastCC[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CCv];];
If[NoLv == 2,
 ScrollEnergyVdWandElastv = EVdWv + fEelastCC[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CCv] +
       fEelastCC[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CBNv];];

Return[ScrollEnergyVdWandElastv];
];

fScrollEnergy[NoLv_, Lwv_, L1v_, RIn1v_, hv_, aCCv_, epsVdWv_, CCv_, CBNv_] := Module[
{ScrollEnergyv = -10^20 eV / atom},
 If[RIn1v / m <= fRIn1Sharp[NoLv, L1v, hv] / m,
ScrollEnergyv =
     fScrollEnergyVdWandElast[NoLv, Lwv, L1v, RIn1v, hv, aCCv, epsVdWv, CCv, CBNv];
"note: the function fScrollEnergyVdWandElast[1,..] is analytycal";
"whereas the function fScrollEnergy[....] uses the 'If[..]'- function";
];
```

```
 If[RIn1v / m >= fRIn1Sharp[NoLv, L1v, hv] / m,
If[NoLv == 1, ScrollEnergyv = fEelastCC[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CCv];];
If[NoLv == 2, ScrollEnergyv = fEelastCC[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CCv] +
        fEelastCC[NoLv, Lwv, L1v, RIn1v, hv, aCCv, CBNv];];

];
Return[ScrollEnergyv];
];

ScrollEnergyp = fScrollEnergy[NoLp, Lwp, L1p, RIn1p, hp, aCCp, epsVdWp, CCp, CBNp];
ScrollEnergyp = fScrollEnergy[1, Lwp, L1p, RIn1p, hp, aCCp, epsVdWp, CCp, CBNp];
Print["fScrollEnergy[1,Lwp,L1p, RIn1p,hp, aCCp, epsVdWp,CCp,CBNp]="];
Print["=fScrollEnergy[1, Lw=", Lwp / nm, "nm, L1=",
  L1p / nm, "nm, RIn1=", RIn1p / nm, "nm, h=", hp / nm, "nm,"];
Print[" aCC=", aCCp / nm, "nm, epsVdW=", epsVdWp / (eV / atom),
  "eV/atom, CC=", CCp / (eV AA ^ 2 / atom), "(eV AA^2/atom)="];
Print["            =", ScrollEnergyp / (eV / atom), "eV/atom"];

Print[" III.5. Determine the inner angles mismatch for the bi-layer nanoscroll
       for the high nanoribbon Length"];
Print[" For L1=", L1p / nm, "nm,RIn=",
  RIn1p / nm, "nm,h=", hp / nm, "nm  and  dPhi12=0:"];
Print[" ScrollEnergy=", ScrollEnergyp / (eV / atom), "eV/atom"];
Print[" For L1=", L1p / nm, "nm,RIn=",
  RIn1p / nm, "nm,h=", hp / nm, "nm  and  dPhi12=Pi:"];
Print[" ScrollEnergy=", ScrollEnergyp / (eV / atom), "eV/atom"];
Print["-------------------------------------------------------------"];

Print[" IV.The potential energy of the nanoscroll"];
Print[" as a function of the inner radius RIn"];
PlotRangep =
 Switch[NoLp, 1, PlotRangeMonoScroll, 2, PlotRangeBiScroll];
RIn1Minp =
 Switch[NoLp, 1, RIn1MinMonoScroll, 2, RIn1MinBiScroll];
RIn1Maxp =
 Switch[NoLp, 1, RIn1MaxMonoScroll, 2, RIn1MaxBiScroll];
PlotRangep =
 Switch[NoLp, 1, PlotRangeMonoScroll, 2, PlotRangeBiScroll];
RIn1Maxp =
 Switch[NoLp, 1, RIn1MaxMonoScroll, 2, RIn1MaxBiScroll];
tL1 = Switch[NoLp, 1, {7. nm, 10. nm, 12.5 nm, 15. nm},
  2, {15. nm, 20. nm, 25. nm, 30. nm}];
Print[" NoL=", NoLp];
Print[" epsVdW=", epsVdWp / (eV / atom),
  "eV/atom, C=", CCp / (eV nm ^ 2 / atom), "(eV nm^2/atom)",
 "(eV nm^2/atom),aCC=", aCCp / nm, "nm,h=", hp / nm, "nm"];
Print[" Plot ScrollEnergy[RIn1/nm]/(eV/atom) for L1=", L1p / nm,
 "nm (NoL=", NoLp, ",Lw=", Lwp / nm, "nm"];
PlotScrollEnergyVsRIn1 =
  Plot[(fScrollEnergy[NoLp, Lwp, L1p, RIn1nmv nm, hp, aCCp, epsVdWp,
    CCp, CBNp]) / (eV /
    atom), {RIn1nmv, RIn1Minp / nm, RIn1Maxp / nm},
   PlotRange -> PlotRangep / (eV / atom)];
Print[PlotScrollEnergyVsRIn1];
Print[" Plot ScrollEnergy[RIn1/nm]/(eV/atom) for L1=", tL1 / nm,
 "nm (NoL=", NoLp, ",w=", Lwp / nm, "nm)"];
PlotScrollEnergyVsRIn1L1th =
```

```
 Plot[(fScrollEnergy[NoLp, Lwp, tL1[[1]], RIn1nmv nm, hp, aCCp, epsVdWp,
    CCp, CBNp] ) / (eV /
    atom), {RIn1nmv, RIn1Minp / nm, RIn1Maxp / nm},
   PlotRange -> PlotRangep / (eV / atom)];
PlotScrollEnergyVsRIn1L2th =
 Plot[(fScrollEnergy[NoLp, Lwp, tL1[[2]], RIn1nmv nm, hp, aCCp, epsVdWp,
    CCp, CBNp] ) / (eV /
    atom), {RIn1nmv, RIn1Minp / nm, RIn1Maxp / nm},
   PlotRange -> PlotRangep / (eV / atom)];
PlotScrollEnergyVsRIn1L3th =
 Plot[(fScrollEnergy[NoLp, Lwp, tL1[[3]], RIn1nmv nm, hp, aCCp, epsVdWp,
    CCp, CBNp] ) / (eV /
    atom), {RIn1nmv, RIn1Minp / nm, RIn1Maxp / nm},
   PlotRange -> PlotRangep / (eV / atom)];
PlotScrollEnergyVsRIn1L4th =
 Plot[(fScrollEnergy[NoLp, Lwp, tL1[[4]], RIn1nmv nm, hp, aCCp, epsVdWp,
    CCp, CBNp]) / (eV /
    atom), {RIn1nmv, RIn1Minp / nm, RIn1Maxp / nm},
   PlotRange -> PlotRangep / (eV / atom)];
Print[Show[{PlotScrollEnergyVsRIn1L1th, PlotScrollEnergyVsRIn1L2th,
  PlotScrollEnergyVsRIn1L3th, PlotScrollEnergyVsRIn1L4th}]];
Print["The examples of using of 'fScrollEnergy[..]' function:"]
Print["fScrollEnergy[NoLp,Lwp,tL1[[1]],RIn1p,hp, aCCp, epsVdWp,CCp, CBNp]=",
  fScrollEnergy[NoLp, Lwp, tL1[[1]], RIn1p, hp, aCCp, epsVdWp, CCp, CBNp] / (eV / atom),
  " eV/atom"];
Print["fScrollEnergy[NoLp,Lwp,tL1[[1]],1nm,hp, aCCp, epsVdWp,CCp, CBNp]=",
  fScrollEnergy[NoLp, Lwp, tL1[[1]], 1 nm, hp, aCCp, epsVdWp, CCp, CBNp] / (eV / atom),
  " eV/atom"];
Print["fScrollEnergy[NoLp,Lwp,7nm,1nm,hp, aCCp, epsVdWp,CCp, CBNp]=",
  fScrollEnergy[NoLp, Lwp, 7. nm, 1. nm, hp, aCCp, epsVdWp, CCp, CBNp] / (eV / atom),
  " eV/atom"];
Print["fEVdWLayer1Overlap[1,Lwp,7.nm,1.nm,hp,aCCp,epsVdWp][[1]]=",
  fEVdWLayer1Overlap[1, Lwp, 7. nm, 1. nm, hp, aCCp, epsVdWp][[1]] / (eV / atom),
  "eV/atom (right !=0 value, because the layer overlaps"];
Print["fEVdWLayer1Overlap[1,Lwp,7.nm,1.5nm,hp,aCCp,epsVdWp][[1]]=",
  fEVdWLayer1Overlap[1, Lwp, 7. nm, 2.5 nm, hp, aCCp, epsVdWp][[1]] / (eV / atom),
  "eV/atom !=0, wrong value of the fEVdWLayer1Overlap[..]
    function because the layer does not not overlap"];
Print[];
Print["The analytical expressions of the fEVdWLayer1Overlap[..] function:"];
Print[];
Print["--- fEVdWLayer1Overlap[NoL1,Lwv,Lpv,RInv,hv,aCCv,epsVdWv][[1]]: ---"];
Print[fEVdWLayer1Overlap[NoL1, Lwv, Lpv, RInv, hv, aCCv, epsVdWv][[1]]];
Print[];
Print["--- fEVdWLayer1Overlap[NoL2,Lwv,Lpv,RInv,hv,aCCv,epsVdWv][[1]]: ---"];
Print[fEVdWLayer1Overlap[NoL2, Lwv, Lpv, RInv, hv, aCCv, epsVdWv][[1]]];
Print[];
Print["The Analytical expression of "];
Print["fScrollEnergyVdWandElast[",
  NoLp, ",Lwv,L1v,RIn1v,hv,aCCv, epsVdWv, CCv,CBNv]:"];
Print[fScrollEnergyVdWandElast[NoLp, Lwv, L1v, RIn1v, hv, aCCv, epsVdWv, CCv, CBNv]];
Print["-----------------------------------------------------------"];

Print["V. Export the data of the plots of the nanoscroll energy"];
Print["   as a function of the inner radius"];
Print["The parameters of the output file"];
Print["The number of the output points = ", npRIn1];
```

```
Print["Export the plot data to the files:"];
tRIn1nmRegular =
  Table[(RIn1Minp + (RIn1Maxp - RIn1Minp) iiRin / (npRIn1)) / nm, {iiRin, 1, npRIn1}];
tScrollEnergy = tRIn1nmRegular;
tScrollEnergyeVatom = tRIn1nmRegular;
tPlotEvsRin = Table[{}, {ii, 1, Length[tL1]}];
AllPlotsEVsRin = {};

For[iiL1 = 1, iiL1 <= Length[tL1], iiL1 ++,
L1pi = tL1[[iiL1]];
NanoscrollNamep =
   StringJoin["Nanoscroll", ToString[NoLp], "L", ToString[L1pi / nm], "nm"];
Print["NanoscrollName=", NanoscrollNamep];
ScrollEnergyFileName = StringJoin["EvsRIn1", NanoscrollNamep, ".dat"];
Print["ScrollEnergyFileName=", ScrollEnergyFileName];

For[iiRIn1 = 1, iiRIn1 <= npRIn1, iiRIn1 ++,
RIn1pi = tRIn1nmRegular[[iiRIn1]] nm;
tScrollEnergy[[iiRIn1]] = fScrollEnergy[NoLp, Lwp, L1pi, RIn1pi, hp, aCCp, epsVdWp,
    CCp, CBNp];

tScrollEnergyeVatom[[iiRIn1]] = (tScrollEnergy[[iiRIn1]]) / (eV / atom);];
tPlotEvsRin[[iiL1]] = ListPlot[Transpose[{tRIn1nmRegular, tScrollEnergyeVatom}],
    PlotRange -> PlotRangep / (eV / atom)];
Print[tPlotEvsRin[[iiL1]]];
AllPlotsEVsRin = Join[{AllPlotsEVsRin, tPlotEvsRin[[iiL1]]}];
CarbonNanoscrollEnergyVsRinFileName = StringJoin[NanoscrollNamep, "dat"];
Export[ToFileName[NotebookDirectory[], ScrollEnergyFileName],
   Transpose[{Insert[tRIn1nmRegular, "RIn1[nm]", 1],
     Insert[tScrollEnergyeVatom, "E[eV/atom]", 1]}]]
];
Print["Plot ScrollEnergy[RIn1/nm]/(eV/atom) for L1=", tL1 / nm,
 "nm (NoL=", NoLp, ",Lw=", Lwp / nm, "nm)"];
Print[Show[AllPlotsEVsRin]];
```

The source of the data of the manuscript

Structure and energetics of carbon, hexagonal boron nitride,

and carbon/hexagonal boron nitride single-layer and bilayer nanoscrolls

/ A.I. Siahlo, N.A. Poklonski, A.V. Lebedev, I.V. Lebedeva, A.M. Popov, S.A. Vyrko, A.A. Knizhnik, Yu.E. Lozovik

// Phys. Rev. Materials.— 2018.— V. 2, № 3.— P. 036001 (9 pp.). [DOI: 10.1103/PhysRevMaterials.2.036001]

I.0 The Units (nm, meV, AA)

I.1. All Input Parameters and Constants--------------

I.1.1. The sampling parameters

npRIn1=1000

I.1.2. The Input Geometry Parameters of the system

The carbon nanoribbon length L1=14.839nm

The carbon nanoribbon width Lw=11.8nm

Number of the layers in carbon nanoscroll NoL=1

The length of a carbon nanoribbon L1=14.839nm

The carbon nanoribbon width Lw=1.nm

The inner radius of the nanoscroll RIn1=1.14nm

I.1.2. The Input Energy Constants

epsVdW - the interlayer interaction energy per one atom of

the nanoscroll:

epsVdW=0.035eV/atom

C - the bending elastic constant:

CCelast=2.01eV AA^2/atom

CCBNelast=2.01eV AA^2/atom

I.1.3.The Input Geometry constants--------------

The interatomic distance aCC and the interlayer distance h

h=0.3354 nm (Interlayer distance)

aCC=0.142nm, h=0.3354nm

NatomsInCell=2

dPhi12 - The difference of the inner angles of the spirales

of the Layers

I.5.The parameters for the visualisation

I.6. The parameters of the output file

NanoscrollName=Nanoscroll1L14.839nm

Nanoscroll1L14.839nm.txt

(The output of the data to a file Is Not Performed)

The number of the output points = 1000

I.7. The Input Numerical Constants used in the programm

The Indexes used for the work with EVdW[...] function

--------End of the Input---------------

II. The derivated parameters and the functions required

II.1. The derivated parameters

The cell area Sa=$\frac{3\sqrt{3}\ \mathrm{aCC}^2}{4}$=0.0261938nm^2

II.2. The required functions--------------

II.2.1. The function fSpiraleLen[1,φIn, φOut, h] defines

the Length of a Spirale with the inner agle φIn and the outer angle φOut(>=φIn):

$$\text{fSpiraleLen[1, }\varphi\text{In, }\varphi\text{Out, h]} = \frac{h\left(-\varphi In\sqrt{1+\varphi In^2} + \varphi Out\sqrt{1+\varphi Out^2} - \text{ArcSinh}[\varphi In] + \text{ArcSinh}[\varphi Out]\right)}{4\pi}.$$

II.2.2. The function fElast[φIn,ρOut] is required to calculate an nanoscrollelastic energy:

$$\text{fElast}[\varphi In,\varphi Out] = \frac{\sqrt{1+\varphi In^2}}{\varphi In} - \frac{\sqrt{1+\varphi Out^2}}{\varphi Out} - \text{ArcSinh}[\varphi In] + \text{ArcSinh}[\varphi Out].$$

II.2.3. Define the function fPhiOutvsPhiInLh[1,φIn,L,h].

The function $\text{fPhiOutvsPhiInLh}[1,\varphi In,L,h] = \sqrt{\frac{4 L \pi}{h} + \varphi In^2}$ is a good approximation to obtain the value of φOut for the defined φIn,L,h.

The inverse function $\text{fPhiInvsPhiOutLh}[1,\varphi Out, L, h]] = \sqrt{-\frac{4 L \pi}{h} + \varphi Out^2}$

could be used in the program applications
if ROut (instead of RIn) is the input parameter of the system.

II.2.4. The functions fSpirale1Under(Over)Spirale1Length[NoLv,PhiIn1v ,PhiOut1v,hv]

These functiona are not required, dut could be helpful),

fSpirale1UnderSpirale1Length[1,PhiIn1v ,PhiOut1v,hv]=

$$=\text{fSpiraleLen[NoLv,PhiIn1v ,PhiOut1v-2Pi,hv]} = \frac{1}{4\pi}$$

$$\text{hv NoLv}\left(-\text{PhiIn1v}\sqrt{1+\text{PhiIn1v}^2} + \sqrt{1+(\text{PhiOut1v}-2\pi)^2}\,(\text{PhiOut1v}-2\pi) - \text{ArcSinh}[\text{PhiIn1v}] + \text{ArcSinh}[\text{PhiOut1v}-2\pi]\right);$$

fSpirale1UnderSpirale1Length[NoLp,PhiIn1p ,PhiOut1p,hp]=fSpirale1UnderSpirale1Length[

$$1, \frac{\text{PhiIn1p}}{2\pi}(2\text{Pi}), \frac{\text{PhiOut1p}}{2\pi}(2\text{Pi}), 0.3354\text{nm}] =$$

$$=0.0266903\left(-\text{PhiIn1p}\sqrt{1+\text{PhiIn1p}^2} + \sqrt{1+(\text{PhiOut1p}-2\pi)^2}\,(\text{PhiOut1p}-2\pi) - \text{ArcSinh}[\text{PhiIn1p}] + \text{ArcSinh}[\text{PhiOut1p}-2\pi]\right)\text{nm}.$$

fSpirale1OverSpirale1Length[1,PhiIn1v ,PhiOut1v,hv]=

$$=\text{fSpiraleLen[NoLv,PhiIn1v+2Pi ,PhiOut1v,hv]} = \frac{1}{4\pi}$$

$$\text{hv NoLv}\left(\text{PhiOut1v}\sqrt{1+\text{PhiOut1v}^2} + (-\text{PhiIn1v}-2\pi)\sqrt{1+(\text{PhiIn1v}+2\pi)^2} + \text{ArcSinh}[\text{PhiOut1v}] - \text{ArcSinh}[\text{PhiIn1v}+2\pi]\right);$$

fSpirale1OverSpirale1Length[NoLp,PhiIn1p ,PhiOut1p,hp]=fSpirale1OverSpirale1Length[

$$1, \frac{\text{PhiIn1p}}{2\pi}(2\text{Pi}), \frac{\text{PhiOut1p}}{2\pi}(2\text{Pi}), 0.3354\text{nm}] =$$

$$=0.0266903\left(\text{PhiOut1p}\sqrt{1+\text{PhiOut1p}^2} + (-\text{PhiIn1p}-2\pi)\sqrt{1+(\text{PhiIn1p}+2\pi)^2} + \text{ArcSinh}[\text{PhiOut1p}] - \text{ArcSinh}[\text{PhiIn1p}+2\pi]\right)\text{nm}.$$

II.2.4. The function fRIn1Sharp[NoLv,L1v,hv]

$$\text{fRIn1Sharp[NoLv,L1v,hv]} = -\frac{\text{hv NoLv}}{2} + \frac{\text{L1v}}{2\pi}$$

is a good approximation to obtain the value of the sharp in the dependence ScrollEnergy[RIn]

fRIn1Sharp[1, 14.839nm, 0.3354nm] = 2.194nm

III. Begin of Calculation

III.1. The inner and the outer angle of the spirale of the layer:

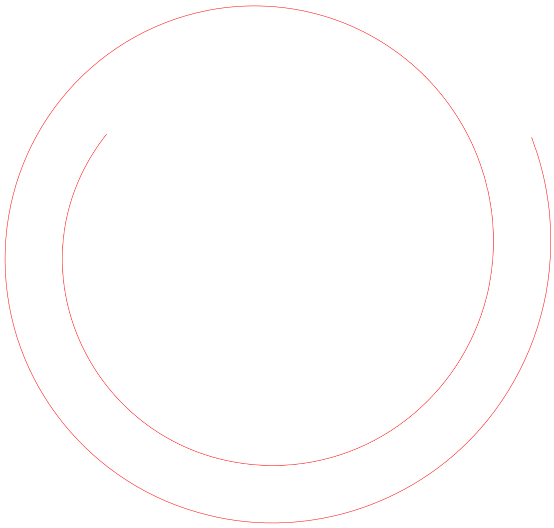
$\varphi In1=\frac{2\,\pi\,RIn1}{h}$, φOut1=fPhiOutvsPhiInLh[1,ϕIn1,L1,h];

For RIn1=1.14nm,h=0.3354nm:

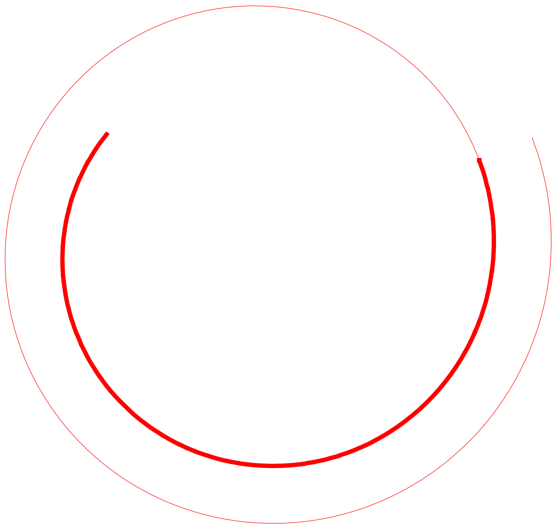
φIn1=3.39893(2Pi),ΨOut1=5.06316(2Pi).

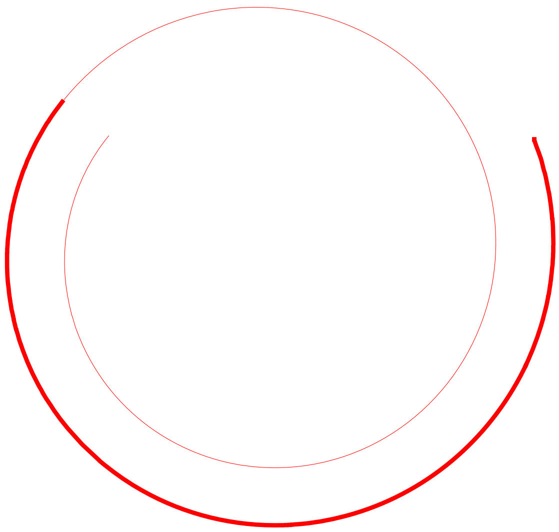
L1=14.839nm, RIn1=1.14nm

Plot the Spirale of the layer:



{Spirale,Spirale1UnderSpirale1},{Spirale1,Spirale1OverSpirale1}:





III.2. The nanoscroll energy calculation

III.2.1. The elastic energy calculation

EelastC=5.7333eV/atom

III.2.2. The Van-der-Waals energy calculation

EVdWvardPhi12allp[[iEVdW]]=-7.91941eV/atom

(EVdWvardPhi12allp[[iEVdW1Un1]]=-3.49244eV/atom

EVdWvardPhi12allp[[iEVdW1Ov1]]=-4.42696eV/atom)

III.4. The total energy of the nanoscroll

fScrollEnergy[1,Lwp,L1p, RIn1p,hp, aCCp, epsVdWp,CCp,CBNp]=

=fScrollEnergy[1, Lw=1.nm, L1=14.839nm, RIn1=1.14nm, h=0.3354nm, aCC=0.142nm, epsVdW=0.035eV/atom, CC=2.01(eV AA^2/atom)=

=-2.18611eV/atom

III.5. Determine the inner angles mismatch for the bi-layer nanoscroll
for the high nanoribbon Length

For L1=14.839nm,RIn=1.14nm,h=0.3354nm and dPhi12=0:

ScrollEnergy=-2.18611eV/atom

For L1=14.839nm,RIn=1.14nm,h=0.3354nm and dPhi12=Pi:

ScrollEnergy=-2.18611eV/atom

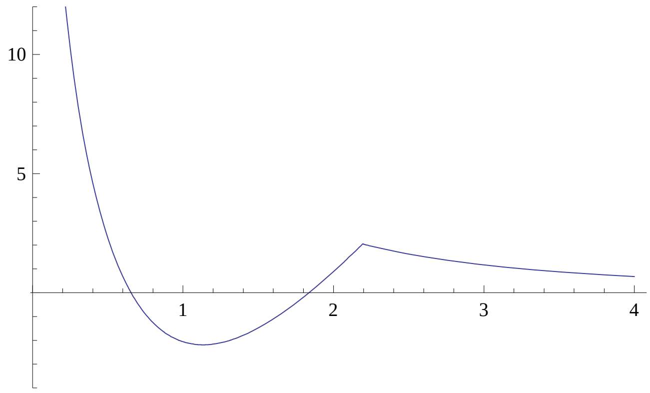
IV.The potential energy of the nanoscroll

as a function of the inner radius RIn

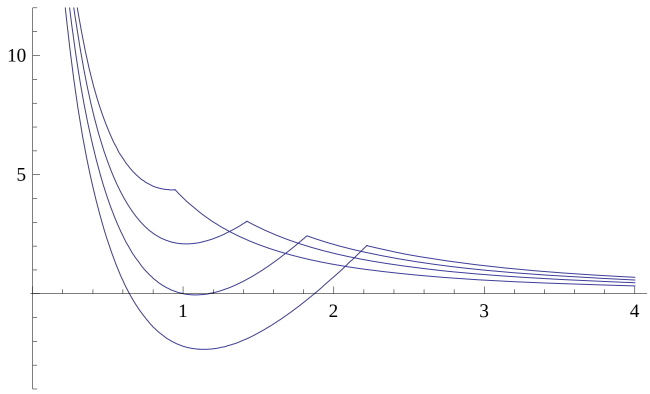
NoL=1

epsVdW=0.035eV/atom, C=0.0201(eV nm^2/atom)(eV nm^2/atom),aCC=0.142nm,h=0.3354nm

Plot ScrollEnergy[RIn1/nm]/(eV/atom) for L1=14.839nm (NoL=1,Lw=1.nm



Plot ScrollEnergy[RIn1/nm]/(eV/atom) for L1={7., 10., 12.5, 15.}nm (NoL=1,w=1.nm)



The examples of using of 'fScrollEnergy[..]' function:

fScrollEnergy[NoLp,Lwp,tL1[[1]],RIn1p,hp, aCCp, epsVdWp,CCp, CBNp]=3.26809 eV/atom

fScrollEnergy[NoLp,Lwp,tL1[[1]],1nm,hp, aCCp, epsVdWp,CCp, CBNp]=4.01569 eV/atom

fScrollEnergy[NoLp,Lwp,7nm,1nm,hp, aCCp, epsVdWp,CCp, CBNp]=4.01569 eV/atom

fEVdWLayer1Overlap[1,Lwp,7.nm,1.nm,hp,aCCp,epsVdWp][[1]]=
0.39374eV/atom (right !=0 value, because the layer overlaps

```
fEVdWLayer1Overlap[1,Lwp,7.nm,1.5nm,hp,aCCp,epsVdWp][[1]]=
 12.2479eV/atom !=0, wrong value of the
   fEVdWLayer1Overlap[..] function because the layer does not not overlap
```

```
The analytical expressions of the fEVdWLayer1Overlap[..] function:
```

```
--- fEVdWLayer1Overlap[NoL1,Lwv,Lpv,RInv,hv,aCCv,epsVdWv][[1]]: ---
```

$$-\frac{1}{6\sqrt{3}\ \mathrm{aCCv}^2\,\pi}\mathrm{epsVdWv\ hv\ Lwv}\left(\sqrt{\frac{4\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{4\,\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}\ \sqrt{1+\frac{4\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{4\,\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}+\left(-2\,\pi-\frac{2\,\pi\,\mathrm{RInv}}{\mathrm{hv}}\right)\sqrt{1+\left(2\,\pi+\frac{2\,\pi\,\mathrm{RInv}}{\mathrm{hv}}\right)^2}-\right.$$
$$\left.\mathrm{ArcSinh}\left[2\,\pi+\frac{2\,\pi\,\mathrm{RInv}}{\mathrm{hv}}\right]+\mathrm{ArcSinh}\left[\sqrt{\frac{4\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{4\,\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}\right]\right)-\frac{1}{6\sqrt{3}\ \mathrm{aCCv}^2\,\pi}\mathrm{epsVdWv\ hv\ Lwv}$$
$$\left(-\frac{2\,\pi\,\mathrm{RInv}\sqrt{1+\frac{4\,\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}}{\mathrm{hv}}+\left(-2\,\pi+\sqrt{\frac{4\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{4\,\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}\right)\sqrt{1+\left(-2\,\pi+\sqrt{\frac{4\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{4\,\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}\right)^2}-\right.$$
$$\left.\mathrm{ArcSinh}\left[\frac{2\,\pi\,\mathrm{RInv}}{\mathrm{hv}}\right]-\mathrm{ArcSinh}\left[2\,\pi-\sqrt{\frac{4\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{4\,\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}\right]\right)$$

```
--- fEVdWLayer1Overlap[NoL2,Lwv,Lpv,RInv,hv,aCCv,epsVdWv][[1]]: ---
```

$$-\frac{1}{3\sqrt{3}\ \mathrm{aCCv}^2\,\pi}$$
$$\mathrm{epsVdWv\ hv\ Lwv}\left(\sqrt{\frac{2\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}\ \sqrt{1+\frac{2\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}+\left(-2\,\pi-\frac{\pi\,\mathrm{RInv}}{\mathrm{hv}}\right)\sqrt{1+\left(2\,\pi+\frac{\pi\,\mathrm{RInv}}{\mathrm{hv}}\right)^2}-\right.$$
$$\left.\mathrm{ArcSinh}\left[2\,\pi+\frac{\pi\,\mathrm{RInv}}{\mathrm{hv}}\right]+\mathrm{ArcSinh}\left[\sqrt{\frac{2\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}\right]\right)-\frac{1}{3\sqrt{3}\ \mathrm{aCCv}^2\,\pi}\mathrm{epsVdWv\ hv\ Lwv}$$
$$\left(-\frac{\pi\,\mathrm{RInv}\sqrt{1+\frac{\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}}{\mathrm{hv}}+\left(-2\,\pi+\sqrt{\frac{2\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}\right)\sqrt{1+\left(-2\,\pi+\sqrt{\frac{2\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}\right)^2}-\right.$$
$$\left.\mathrm{ArcSinh}\left[\frac{\pi\,\mathrm{RInv}}{\mathrm{hv}}\right]-\mathrm{ArcSinh}\left[2\,\pi-\sqrt{\frac{2\,\mathrm{Lpv}\,\pi}{\mathrm{hv}}+\frac{\pi^2\,\mathrm{RInv}^2}{\mathrm{hv}^2}}\right]\right)$$

The Analytical expression of

fScrollEnergyVdWandElast[1,Lwv,L1v,RIn1v,hv,aCCv, epsVdWv, CCv,CBNv]:

$$\frac{8\,\mathrm{CCv}\,\mathrm{Lwv}\,\pi\left(\frac{\mathrm{hv}\sqrt{1+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}}{2\pi\,\mathrm{RIn1v}}-\frac{\sqrt{1+\frac{4\,\mathrm{L1v}\,\pi}{\mathrm{hv}}+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}}{\sqrt{\frac{4\,\mathrm{L1v}\,\pi}{\mathrm{hv}}+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}}-\mathrm{ArcSinh}\left[\frac{2\pi\,\mathrm{RIn1v}}{\mathrm{hv}}\right]+\mathrm{ArcSinh}\left[\sqrt{\frac{4\,\mathrm{L1v}\,\pi}{\mathrm{hv}}+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}\right]\right)}{3\sqrt{3}\,\mathrm{aCCv}^2\,\mathrm{hv}}-$$

$$\frac{1}{6\sqrt{3}\,\mathrm{aCCv}^2\,\pi}\mathrm{epsVdWv}\,\mathrm{hv}\,\mathrm{Lwv}$$

$$\left(\sqrt{\frac{4\,\mathrm{L1v}\,\pi}{\mathrm{hv}}+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}\sqrt{1+\frac{4\,\mathrm{L1v}\,\pi}{\mathrm{hv}}+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}+\left(-2\pi-\frac{2\pi\,\mathrm{RIn1v}}{\mathrm{hv}}\right)\sqrt{1+\left(2\pi+\frac{2\pi\,\mathrm{RIn1v}}{\mathrm{hv}}\right)^2}-\right.$$

$$\left.\mathrm{ArcSinh}\left[2\pi+\frac{2\pi\,\mathrm{RIn1v}}{\mathrm{hv}}\right]+\mathrm{ArcSinh}\left[\sqrt{\frac{4\,\mathrm{L1v}\,\pi}{\mathrm{hv}}+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}\right]\right)-\frac{1}{6\sqrt{3}\,\mathrm{aCCv}^2\,\pi}\mathrm{epsVdWv}\,\mathrm{hv}\,\mathrm{Lwv}$$

$$\left(-\frac{2\pi\,\mathrm{RIn1v}\sqrt{1+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}}{\mathrm{hv}}+\left(-2\pi+\sqrt{\frac{4\,\mathrm{L1v}\,\pi}{\mathrm{hv}}+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}\right)\sqrt{1+\left(-2\pi+\sqrt{\frac{4\,\mathrm{L1v}\,\pi}{\mathrm{hv}}+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}\right)^2}-\right.$$

$$\left.\mathrm{ArcSinh}\left[\frac{2\pi\,\mathrm{RIn1v}}{\mathrm{hv}}\right]-\mathrm{ArcSinh}\left[2\pi-\sqrt{\frac{4\,\mathrm{L1v}\,\pi}{\mathrm{hv}}+\frac{4\pi^2\,\mathrm{RIn1v}^2}{\mathrm{hv}^2}}\right]\right)$$

V. Export the data of the plots of the nanoscroll energy

as a function of the inner radius

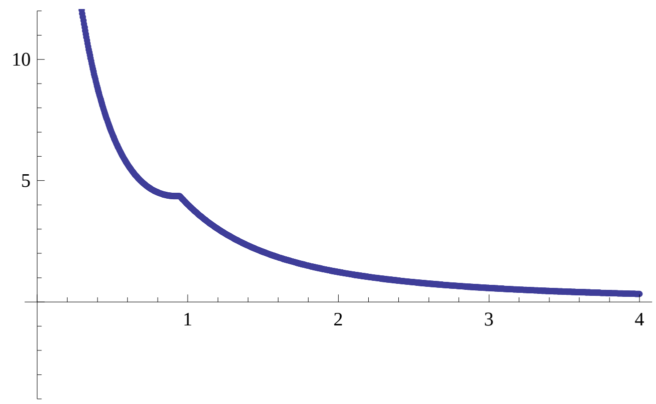
The parameters of the output file

The number of the output points = 1000

Export the plot data to the files:

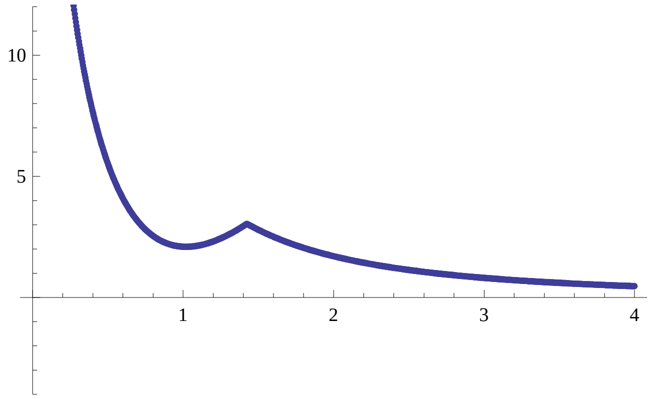
NanoscrollName=Nanoscroll1L7.nm

ScrollEnergyFileName=EvsRIn1Nanoscroll1L7.nm.dat



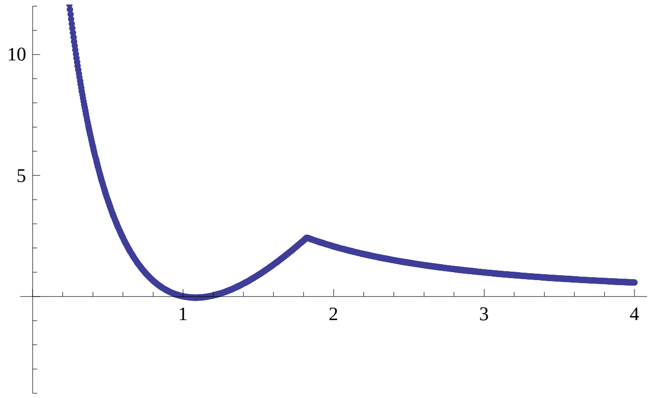
NanoscrollName=Nanoscroll1L10.nm

ScrollEnergyFileName=EvsRIn1Nanoscroll1L10.nm.dat



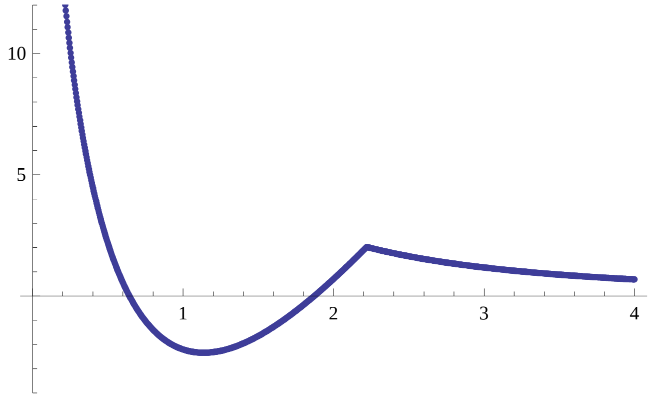
NanoscrollName=Nanoscroll1L12.5nm

ScrollEnergyFileName=EvsRIn1Nanoscroll1L12.5nm.dat

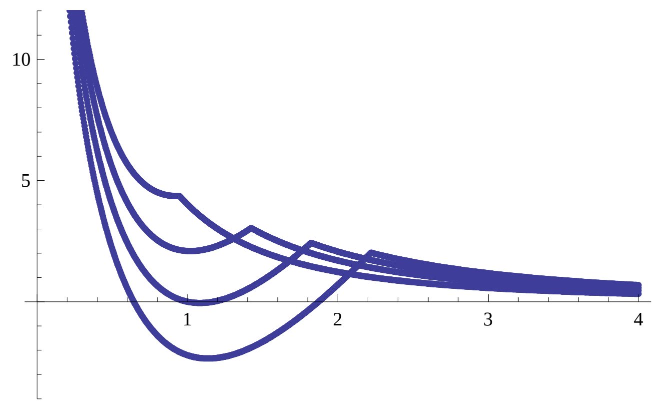


NanoscrollName=Nanoscroll1L15.nm

ScrollEnergyFileName=EvsRIn1Nanoscroll1L15.nm.dat



Plot ScrollEnergy[RIn1/nm]/(eV/atom) for L1={7., 10., 12.5, 15.}nm (NoL=1,Lw=1.nm)


10
5
1
2
3
4