```
In[1]:= Print["  Figure3cd(Layers2L30nmRIn2d1nm.m"];
        Print[];
        Print["   The source of the data of the manuscript"];
        Print["   'Structure and energetics of carbon, "];
        Print["   hexagonal boron nitride, and"];
        Print["   carbon/hexagonal boron nitride"];
        Print["   single-layer and bilayer nanoscrolls' "];
        Print[" / A.I. Siahlo, N.A. Poklonski, A.V. Lebedev,"];
        Print[" I.V. Lebedeva, A.M. Popov, S.A. Vyrko, "];
        Print[" A.A. Knizhnik, Yu.E. Lozovik "];
        Print[" // Phys. Rev. Materials.— 2018.— V. 2,"];
        Print[" № 3.— P. 036001 (9 pp.)."];
        Print[" [DOI: 10.1103/PhysRevMaterials.2.036001] "];
        Print[" ----------------------------------------------------"];

        NoL1 = 1; NoL2 = 2;
        NoLp = NoL2;
        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 = L129d678nm;

        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 = RIn1d14nm;
RIn1p = RIn2d1nm;
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.4.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.5. The parameters of visualization that depend on NoL=", NoLp];
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[" 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 Pi 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, but 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]];
 Print["Manipulating of Spirale1Plot for the different RIn1 and L:"];
 Manipulate[PolarPlot[(Phiv) NoLp hp / (2 Pi) / nm,
   {Phiv, fPhiIn1[NoLp, RIn1nmm nm, hp], fPhiOut1[NoLp, L1nmm nm, RIn1nmm nm, hp]},
   PlotRange → {{-1.1 ROut1p / nm, 1.1 ROut1p / nm}, {-1.1 ROut1p / nm, 1.1 ROut1p / nm}},
   PlotStyle → {Red, Thin}, Axes → None], {{RIn1nmm, RIn1p / nm}, RIn1Minp / nm, RIn1Maxp / nm},
  {{L1nmm, L1p / nm}, 0.5 tL1[[1]] / nm, 1.5 tL1[[Length[tL1]]] / nm}]]
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,
     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"];
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]];

Print[];
Print["Manipulating of the plot of the nanoscroll energy as the functoon"];
Print[" of the nanoscroll inner radius:"];
Print[" "];
Print["(Manipulate[Plot[fScrollEnergy[...,L1nmm,RIn1,hp,...]]],"];
Print["                        where L1nmm (is L1 in nanometers) "];
Print["                        is the manipulated value"];
Print["                       )"];
Manipulate[Plot[
  (fScrollEnergy[NoLp, Lwp, L1nmm nm, RIn1nmv nm, hp, aCCp, epsVdWp, CCp, CBNp]) / (eV / atom),
  {RIn1nmv, RIn1Minp / nm, RIn1Maxp / nm}, PlotRange → PlotRangep / (eV / atom)],
 {{L1nmm, L1p / nm}, 0.5 tL1[[1]] / nm, 1.5 tL1[[Length[tL1]]] / nm}]
```

Figure3cd(Layers2L30nmRIn2d1nm.m

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,

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 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=29.678nm
 The carbon nanoribbon width Lw=11.8nm
-----------------------------------------------------------
 Number of the layers in carbon nanoscroll NoL=2
 The length of a carbon nanoribbon L1=29.678nm
 The carbon nanoribbon width Lw=1.nm
 The inner radius of the nanoscroll RIn1=2.1nm
 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.4.The parameters for the visualisation
 I.5. The parameters of visualization that depend on NoL=2
 I.6. The parameters of the output file
 NanoscrollName=Nanoscroll2L29.678nm
Nanoscroll2L29.678nm.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 $Sa=\frac{3\sqrt{3}\ aCC^2}{4}=0.0261938nm\hat{}2$

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

II.2.1. The function fSpiraleLen[2,φIn, φOut, h] defines

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

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

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

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

II.2.3. Define the function fPhiOutvsPhiInLh[2,φIn,L,h].

The function $fPhiOutvsPhiInLh[2,\varphi In,L,h]=\sqrt{\frac{2\,L\,\pi}{h}+\varphi In^2}$ is a

good approximation to obtain the value of φOut for the defined φIn,L,h.

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

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, but could be helpful),

fSpirale1UnderSpirale2Length[1,PhiIn1v ,PhiOut1v,hv,dPhi12v]=

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

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

fSpirale1UnderSpirale2Length[NoLp,PhiIn1p,PhiOut1p,hp,dPhi12p]=fSpirale1UnderSpirale2Length[

$$2,\frac{PhiIn1p}{2\pi}(2Pi),\frac{PhiOut1p}{2\pi}(2Pi),0.3354nm,0.25(2Pi)]\ =$$

$$=0.0533806\left(-PhiIn1p\sqrt{1+PhiIn1p^2}+\right.$$
$$\left.\sqrt{1+(PhiOut1p-\pi)^2}\ (PhiOut1p-\pi)-ArcSinh[PhiIn1p]+ArcSinh[PhiOut1p-\pi]\right)nm.$$

fSpirale1OverSpirale2Length[1,PhiIn1v ,PhiOut1v,hv,dPhi12v]=

$$=\text{fSpiraleLen[NoLv,PhiIn1v+Pi ,PhiOut1v,hv]}=\frac{1}{4\pi}\,\text{hv NoLv}\left(\text{PhiOut1v}\sqrt{1+\text{PhiOut1v}^2}+(-\text{PhiIn1v}-\pi)\sqrt{1+(\text{PhiIn1v}+\pi)^2}+\text{ArcSinh[PhiOut1v]}-\text{ArcSinh[PhiIn1v}+\pi]\right);$$

$$\text{fSpirale1OverSpirale2Length[NoLp,PhiIn1p ,PhiOut1p,hp]=fSpirale1OverSpirale1Length[}2,\frac{\text{PhiIn1p}}{2\pi}\text{(2Pi)},\frac{\text{PhiOut1p}}{2\pi}\text{(2Pi),0.3354nm]}=$$

$$=0.0533806\left((-4.71239-\text{PhiIn1p})\sqrt{1+(4.71239+\text{PhiIn1p})^2}+\text{PhiOut1p}\sqrt{1+\text{PhiOut1p}^2}-\text{ArcSinh[4.71239}+\text{PhiIn1p]}+\text{ArcSinh[PhiOut1p]}\right)\text{nm}.$$

fSpirale2UnderSpirale1Length[1,PhiIn1v ,PhiOut1v,hv]=

$$\text{fSpiraleLen[NoLv,PhiIn1v, PhiOut1v -2 Pi/NoLv,hv]}=\frac{1}{4\pi}\,\text{hv}\left(-\text{PhiIn1v}\sqrt{1+\text{PhiIn1v}^2}+\sqrt{1+(\text{PhiOut1v}-2\pi)^2}\,(\text{PhiOut1v}-2\pi)-\text{ArcSinh[PhiIn1v]}+\text{ArcSinh[PhiOut1v}-2\pi]\right);$$

$$\text{fSpirale2UnderSpirale1Length[NoLp,PhiIn1p,PhiOut1p,hp,dPhi12p]=fSpirale2UnderSpirale1Length[}2,\frac{\text{PhiIn1p}}{2\pi}\text{(2Pi)},\frac{\text{PhiOut1p}}{2\pi}\text{(2Pi),0.3354nm,0.25(2Pi)]}=$$

$$=0.0533806\left(-\text{PhiIn1p}\sqrt{1+\text{PhiIn1p}^2}+\sqrt{1+(\text{PhiOut1p}-\pi)^2}\,(\text{PhiOut1p}-\pi)-\text{ArcSinh[PhiIn1p]}+\text{ArcSinh[PhiOut1p}-\pi]\right)\text{nm}.$$

fSpirale1OverSpirale2Length[1,PhiIn1v ,PhiOut1v,hv]=

$$=\text{fSpiraleLen[NoLv,PhiIn1v+Pi ,PhiOut1v,hv]}=\frac{1}{4\pi}\,\text{hv NoLv}\left(\text{PhiOut1v}\sqrt{1+\text{PhiOut1v}^2}+(-\text{PhiIn1v}-\pi)\sqrt{1+(\text{PhiIn1v}+\pi)^2}+\text{ArcSinh[PhiOut1v]}-\text{ArcSinh[PhiIn1v}+\pi]\right);$$

$$\text{fSpirale1OverSpirale2Length[NoLp,PhiIn1p ,PhiOut1p,hp]=fSpirale1OverSpirale2Length[}2,\frac{\text{PhiIn1p}}{2\pi}\text{(2Pi)},\frac{\text{PhiOut1p}}{2\pi}\text{(2Pi),0.3354nm]}=$$

$$=0.0533806\left((-4.71239-\text{PhiIn1p})\sqrt{1+(4.71239+\text{PhiIn1p})^2}+\text{PhiOut1p}\sqrt{1+\text{PhiOut1p}^2}-\text{ArcSinh[4.71239}+\text{PhiIn1p]}+\text{ArcSinh[PhiOut1p]}\right)\text{nm}.$$

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[2, 29.678nm, 0.3354nm] = 4.388nm

III. Begin of Calculation

III.1. The inner and the outer angles of the spirales of the layers:

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

For RIn1=2.1nm,h=0.3354nm:

φIn1=3.13059(2Pi),ΨOut1=4.88707(2Pi).

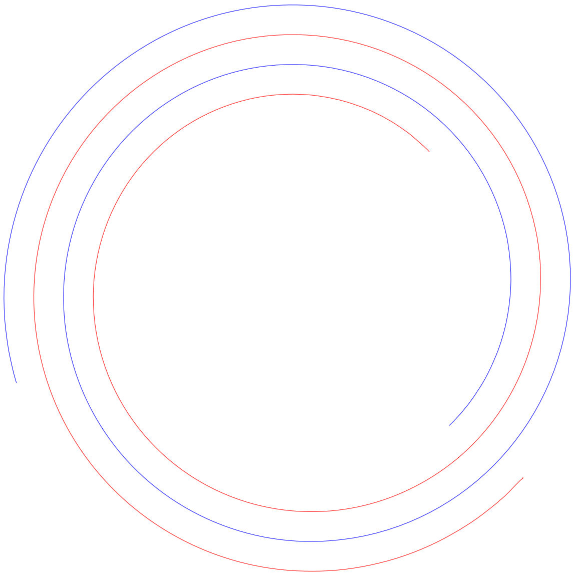
φIn2=3.38059(2Pi),φOut2=5.05087(2Pi)

for dφ12=Pi: PhiIn2=3.63059(2Pi),φOut2=5.2215(2Pi)

L1=29.678nm, RIn1=2.1nm

Plot Spirales of the layers:

Plot the Spirale of the layers:

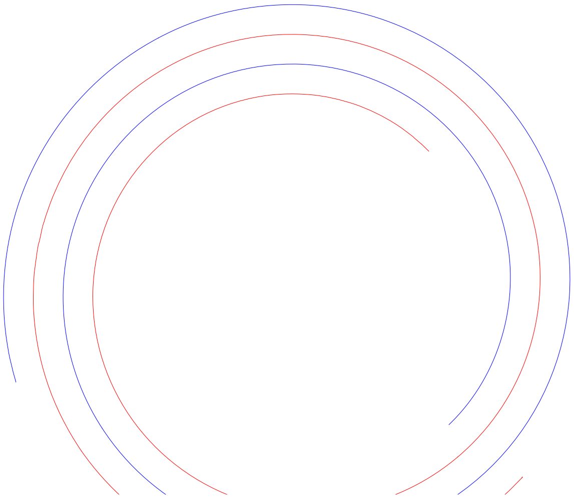


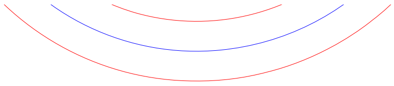
Plot Spirales for dPhi12=Pi (could be NotRequired, dPhi12=0 in this program)

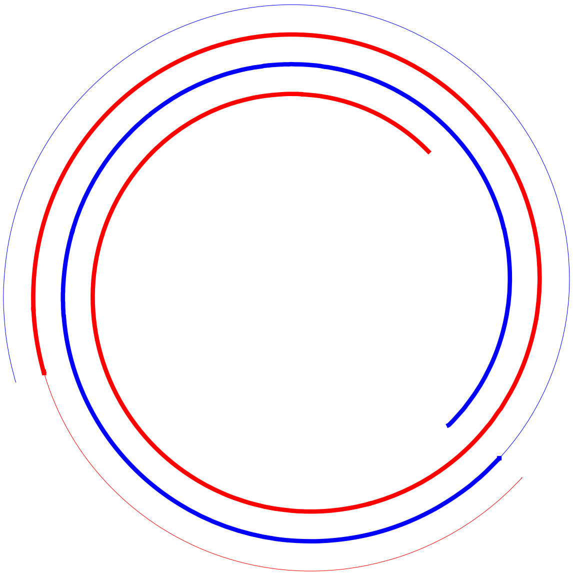
{Spirale1,Spirale2,Spirale1UnderSpirale2,Spirale2UnderSpirale1},

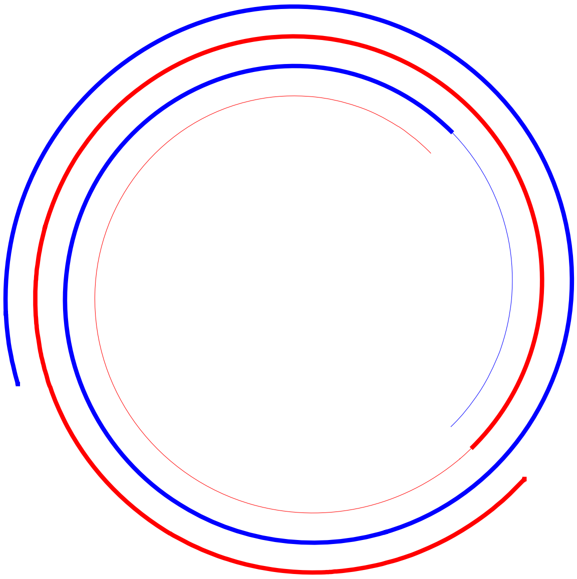
{Spirale1,Spirale2,Spirale1OverSpirale2,Spirale2OverSpirale1}

for dPhi12=0:

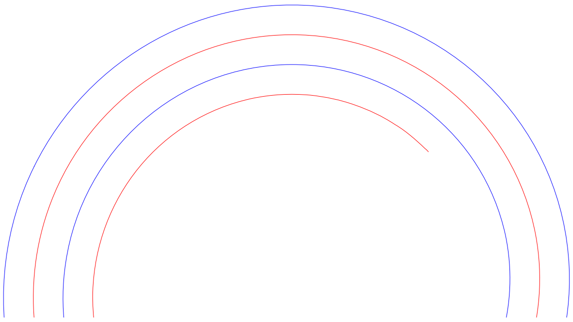


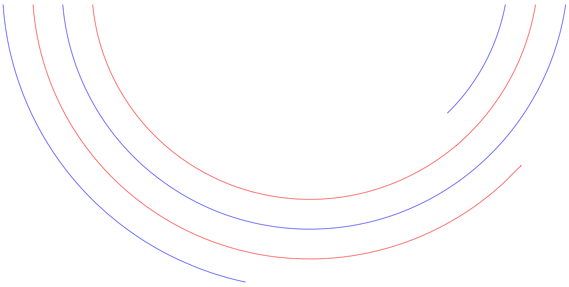


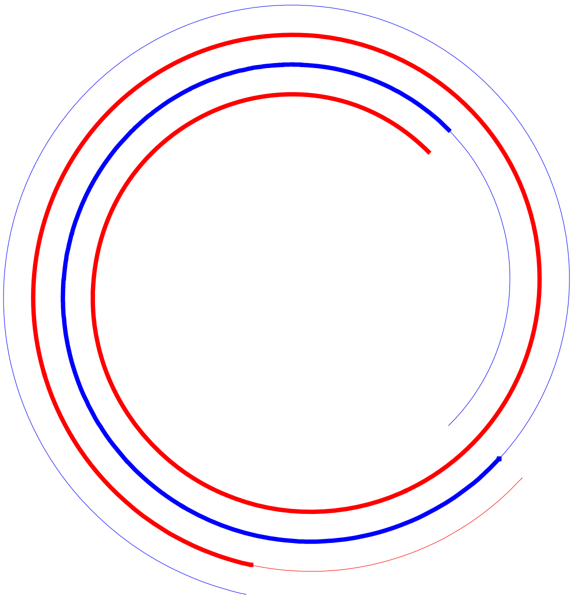


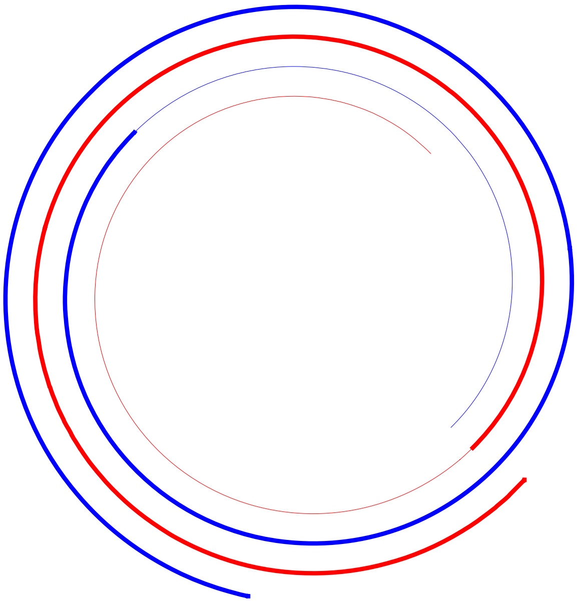


```
for dPhi12=Pi:
```









III.2. The nanoscroll energy calculation

III.2.1. The elastic energy calculation

```
EelastC=6.40779eV/atom
```

EelastBN=6.40779eV/atom

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

for dPhi12=0.5Pi EVdWvardPhi12allp[[iEVdW]]=-55.1954eV/atom

For dPhi12=0.Pi:

EVdWvardPhi12allp[[iEVdW]]=-56.7797eV/atom

EVdWvardPhi12allp[[iEVdW1Un2]]=-13.3111eV/atom

EVdWvardPhi12allp[[iEVdW1Ov2]]=-15.0787eV/atom

EVdWvardPhi12allp[[iEVdW2Un1]]=-13.3111eV/atom

EVdWvardPhi12allp[[iEVdW2Ov2]]=-15.0787eV/atom

For dPhi12=1.Pi:

EVdWvatdPhi12allp[[iEVdW]]=-53.3618eV/atom

EVdWvatdPhi12allp[[iEVdW1Un2]]=-17.6025eV/atom

EVdWvatdPhi12allp[[iEVdW1Ov2]]=-9.61051eV/atom

EVdWvatdPhi12allp[[iEVdW2Un1]]=-8.54618eV/atom

EVdWvatdPhi12allp[[iEVdW2Ov2]]=-17.6025eV/atom

EVdWdPhi12eq0allp=$\left\{-56.7797, \frac{2\,\text{atom}}{\text{eV}}, \frac{3\,\text{atom}}{\text{eV}}, -13.3111, -15.0787, -13.3111, -15.0787\right\}$eV/atom

EVdWEVdWdPhi12eqPip=-55.1954eV/atom

III.3. The energy of flat planes

EnergyFlatPlanes=-eps width/Sa L1(NoL-1) =-39.6556eV/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=29.678nm, RIn1=2.1nm, h=0.3354nm,

aCC=0.142nm, epsVdW=0.035eV/atom, CC=2.01(eV AA^2/atom)=

=-15.3963eV/atom

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

For L1=29.678nm,RIn=2.1nm,h=0.3354nm and dPhi12=0:

ScrollEnergy=-15.3963eV/atom

For L1=29.678nm,RIn=2.1nm,h=0.3354nm and dPhi12=Pi:

ScrollEnergy=-15.3963eV/atom

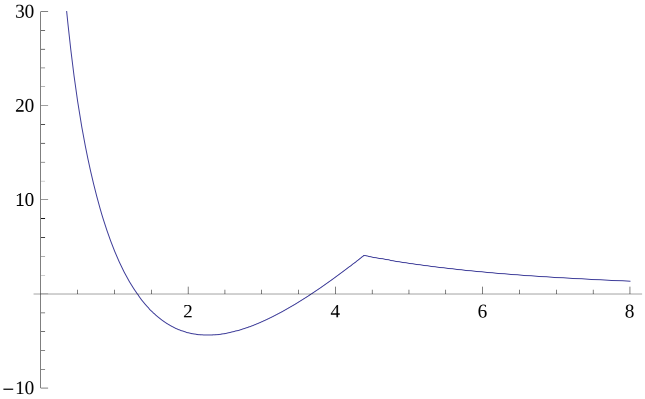
IV.The potential energy of the nanoscroll

as a function of the inner radius RIn

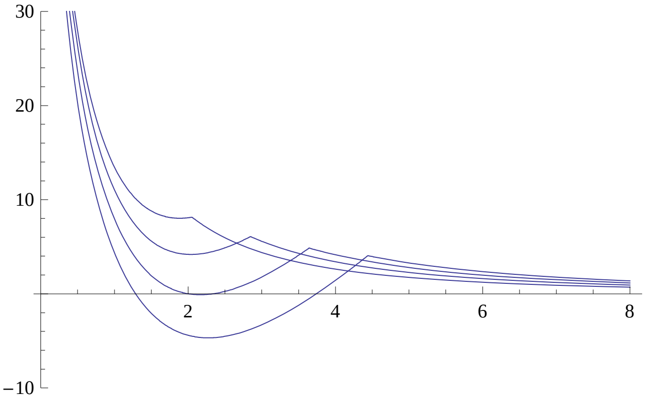
NoL=2

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=29.678nm (NoL=2,Lw=1.nm



Plot ScrollEnergy[RIn1/nm]/(eV/atom) for L1={15., 20., 25., 30.}nm (NoL=2,w=1.nm)



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

fScrollEnergy[NoLp,Lwp,tL1[[1]],RIn1p,hp, aCCp, epsVdWp,CCp,CBNp]=7.85611 eV/atom

fScrollEnergy[NoLp,Lwp,tL1[[1]],1nm,hp, aCCp, epsVdWp,CCp, CBNp]=13.4436 eV/atom

fScrollEnergy[NoLp,Lwp,7nm,1nm,hp, aCCp, epsVdWp,CCp, CBNp]=13.1901 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]]: ---

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

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

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

The Analytical expression of

fScrollEnergyVdWandElast[2,Lwv,L1v,RIn1v,hv,aCCv, epsVdWv, CCv,CBNv]:

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

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

$$\frac{1}{3\sqrt{3}\ \text{aCCv}^2\ \pi}\text{epsVdWv}\ \text{hv}\ \text{Lwv}\left(\sqrt{\frac{2\ \text{L1v}\ \pi}{\text{hv}}+\frac{\pi^2\ \text{RIn1v}^2}{\text{hv}^2}}\ \sqrt{1+\frac{2\ \text{L1v}\ \pi}{\text{hv}}+\frac{\pi^2\ \text{RIn1v}^2}{\text{hv}^2}}\ +\right.$$

$$\left.\left(-2\ \pi-\frac{\pi\ \text{RIn1v}}{\text{hv}}\right)\sqrt{1+\left(2\ \pi+\frac{\pi\ \text{RIn1v}}{\text{hv}}\right)^2}-\text{ArcSinh}\left[2\ \pi+\frac{\pi\ \text{RIn1v}}{\text{hv}}\right]+\text{ArcSinh}\left[\sqrt{\frac{2\ \text{L1v}\ \pi}{\text{hv}}+\frac{\pi^2\ \text{RIn1v}^2}{\text{hv}^2}}\right]\right)-$$

$$\frac{1}{3\sqrt{3}\ \text{aCCv}^2\ \pi}\text{epsVdWv}\ \text{hv}\ \text{Lwv}\left(-\frac{\pi\ \text{RIn1v}\sqrt{1+\frac{\pi^2\ \text{RIn1v}^2}{\text{hv}^2}}}{\text{hv}}+\left(-2\ \pi+\sqrt{\frac{2\ \text{L1v}\ \pi}{\text{hv}}+\frac{\pi^2\ \text{RIn1v}^2}{\text{hv}^2}}\right)\right.$$

$$\left.\sqrt{1+\left(-2\ \pi+\sqrt{\frac{2\ \text{L1v}\ \pi}{\text{hv}}+\frac{\pi^2\ \text{RIn1v}^2}{\text{hv}^2}}\right)^2}-\text{ArcSinh}\left[\frac{\pi\ \text{RIn1v}}{\text{hv}}\right]-\text{ArcSinh}\left[2\ \pi-\sqrt{\frac{2\ \text{L1v}\ \pi}{\text{hv}}+\frac{\pi^2\ \text{RIn1v}^2}{\text{hv}^2}}\right]\right)$$

```
----------------------------------------------------------

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

   as a function of the inner radius

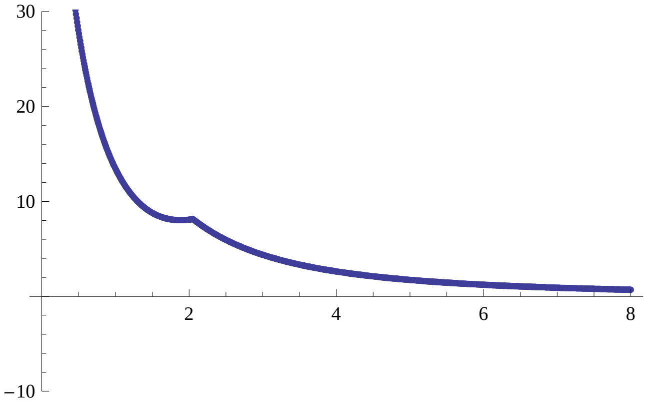
The parameters of the output file

The number of the output points = 1000

Export the plot data to the files:

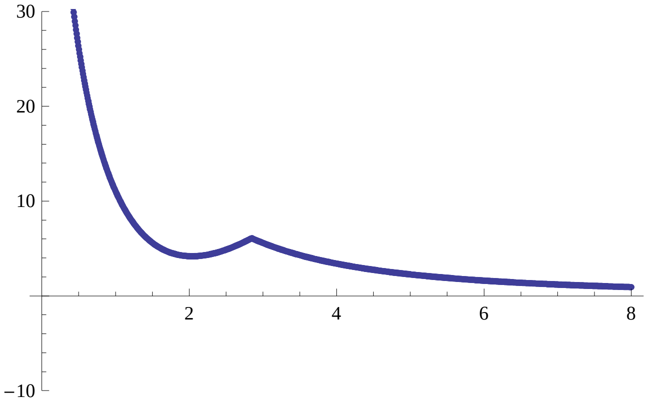
NanoscrollName=Nanoscroll2L15.nm

ScrollEnergyFileName=EvsRIn1Nanoscroll2L15.nm.dat
```



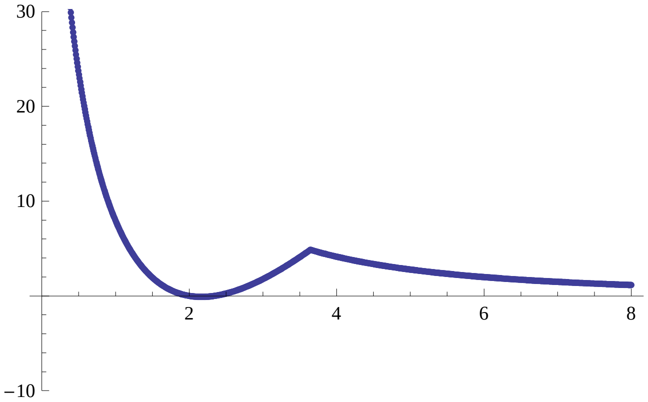
```
NanoscrollName=Nanoscroll2L20.nm
```

```
ScrollEnergyFileName=EvsRIn1Nanoscroll2L20.nm.dat
```



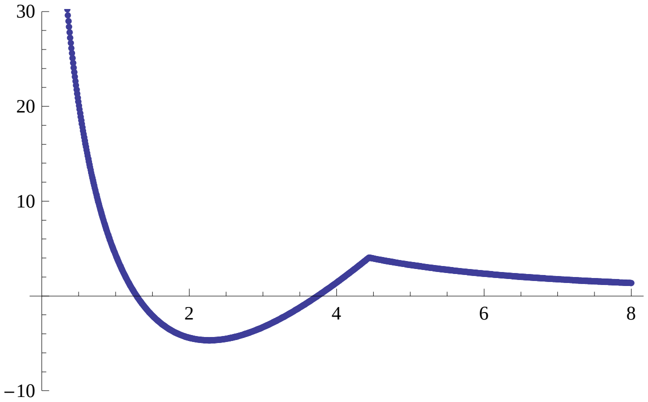
```
NanoscrollName=Nanoscroll2L25.nm

ScrollEnergyFileName=EvsRIn1Nanoscroll2L25.nm.dat
```

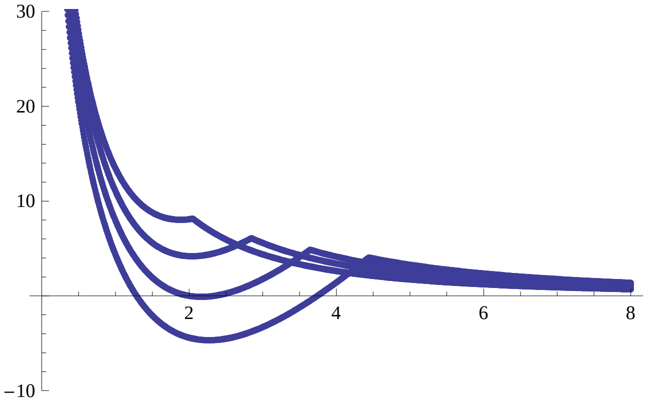


```
NanoscrollName=Nanoscroll2L30.nm

ScrollEnergyFileName=EvsRIn1Nanoscroll2L30.nm.dat
```



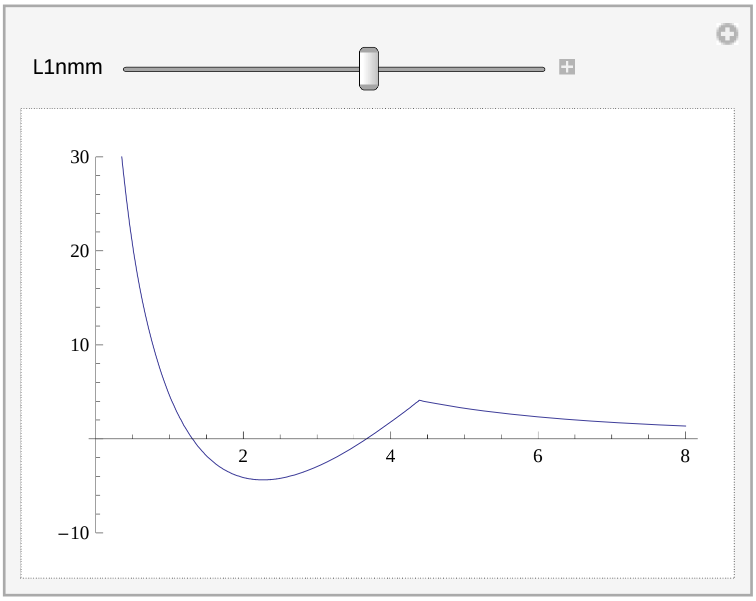
```
Plot ScrollEnergy[RIn1/nm]/(eV/atom) for L1={15., 20., 25., 30.}nm (NoL=2,Lw=1.nm)
```



```
Manipulating of the plot of the nanoscroll energy as the functoon
 of the nanoscroll inner radius:

(Manipulate[Plot[fScrollEnergy[...,L1nmm,RIn1,hp,...]]],
                             where L1nmm (is L1 in nanometers)
                             is the manipulated value
                            )
```

Out[278]=


L1nmm
30
20
10
−10
2
4
6
8