

Supplementary Information: Chiraltube, rolling 2d materials into chiral nanotubes

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1 2D materials

- graphene

nat=2

```
CELL_PARAMETERS (angstrom)
  2.459512147  0.000000000  0.000000000
 -1.229756073  2.130000000  0.000000000
  0.000000000  0.000000000 10.000000000
```

```
ATOMIC_POSITIONS (angstrom)
C 1.229756073  0.71  5.0
C 0.000000000  1.42  5.0
```

- Phosphorene

nat=4

```
CELL_PARAMETERS (angstrom)
  4.62000  0.00000  0.00000
  0.00000  3.30000  0.00000
  0.00000  0.00000 10.00000
```

```
ATOMIC_POSITIONS (angstrom)
P 0.0000 0.00 3.93
P 1.1088 3.30 6.07
P 2.5872 1.65 6.07
P 3.1416 1.65 3.93
```

- MoS₂

nat=3

```
CELL_PARAMETERS (angstrom)
```

```
3.181079696 0.000000000 0.000000000
-1.590540237 2.754889038 0.000000000
0.000000000 0.000000000 10.000000000
```

ATOMIC_POSITIONS (angstrom)

```
S 1.5905260315876495465 0.9182342920325894154 6.565586833
S 1.5905260315876495465 0.9182342920325894154 3.434413167
Mo 0.0000142401699290626 1.8365313040729291692 5.00000000000
```

- Ti_3C_2

nat=5

CELL_PARAMETERS (angstrom)

```
3.0700 0.00000 0.00000
-1.5350 2.65900 0.00000
0.00000 0.00000 15.13100
```

ATOMIC_POSITIONS (angstrom)

```
C 0.000000000 1.7724623240 6.264234069
C 1.535043586 0.8861571658 8.866765931
Ti 1.535043586 0.8861571658 5.192959623
Ti 0.000000000 1.7724623240 9.938040377
Ti 0.000000000 0.000000000 7.565500000
```

2 Special XYZ format

Example of input file for MoS_2

```
3
####1 row with text####
S 1.5905260315876495465 0.9182342920325894154 6.565586833
S 1.5905260315876495465 0.9182342920325894154 3.434413167
Mo 0.0000142401699290626 1.8365313040729291692 5.000000000000
alat
1.0
mass S 28.09
mass Mo 95.95
supercell
3.181079696 0.000000000 0.000000000
-1.590540237 2.754889038 0.000000000
0.000000000 0.000000000 10.000000000
cartesian coordinates
```

Example of output file in special *.xyz format for MoS_2 NT(8,4).

NT (n,m) =(8,4). z=14.5775058, r=5.358011. T (x,y)=(4,5)

S	6.750006046473265	1.5406572141585868	1.3882707683979134
S	3.6973386564148045	0.8439002031959805	1.3882707683979134
S	6.535062662626825	2.2867361619796274	4.512022007241599
S	3.5796026904668525	1.2525674718656548	4.512022007241599
Mo	5.358010951160183	4.066422065634832e-05	4.859115333668328
S	4.895713062587455	4.895732824386468	2.4295211813458093
S	2.681643398893984	2.6816542234862744	2.4295211813458093
Mo	4.827384694754795	2.324787810371771	2.7766145077725364
S	2.286709782895769	6.5350718930837575	0.34702035545001864
S	1.2525530226331951	3.579607746480876	0.34702035545001864
Mo	3.3406379973584603	4.189083327532513	0.6941136818767462
S	6.923597784260712	2.7289008258031143e-05	9.718274071981078
S	3.792424118285034	1.4947646629199356e-05	9.718274071981078
S	6.237935867908364	3.0040576537122012	7.635773246085286
S	3.4168504830753976	1.6454827466372508	7.635773246085286
Mo	5.324315855471739	0.5999516860366897	7.982866572512014
S	4.316777224026051	5.413098990143675	5.553272420189495
S	2.364529333993942	2.965043291733801	5.553272420189495
Mo	4.536735114216091	2.8506693701383075	5.900365746616224
S	1.5406299674524693	6.75001226534826	3.4707715942937054
S	0.8438852787204918	3.6973420628246294	3.4707715942937054
Mo	2.85060050739085	4.5367783835745215	3.817864920720433
S	-1.5406572141585846	6.750006046473266	1.3882707683979147
S	-0.8439002031959791	3.697338656414805	1.3882707683979147
Mo	0.599870868979052	5.324324961434673	1.735364094824642
S	6.880059960253494	0.7752297867608295	12.842025310824766
S	3.768576127837354	0.42463473935591434	12.842025310824766
S	5.862362258998291	3.683600823004169	10.759524484928974
S	3.2111287677181264	2.0177048174365138	10.759524484928974
Mo	5.223663415966982	1.1923178565693706	11.1066178113557
S	3.683554610484816	5.862391296266447	8.677023659033182
S	2.017679504372638	3.2111446729800317	8.677023659033182
Mo	4.189032620008876	3.340701582438573	9.02411698545991
S	0.7751755519244621	6.880066071097221	6.594522833137392
S	0.4246050320407438	3.768579475072687	6.594522833137392
Mo	2.3247145359586825	4.827419981802747	6.94161615956412
S	-2.28673616197963	6.535062662626825	4.512022007241602
S	-1.2525674718656563	3.579602690466852	4.512022007241602
Mo	-4.066422065739496e-05	5.358010951160183	4.8591153336683295
S	-4.895732824386468	4.895713062587455	2.4295211813458115
S	-2.6816542234862744	2.681643398893984	2.4295211813458115
Mo	-2.3247878103717707	4.827384694754795	2.7766145077725386
S	-6.535071893083757	2.286709782895769	0.3470203554500193
S	-3.5796077464808755	1.2525530226331953	0.3470203554500193
Mo	-4.189083327532513	3.3406379973584603	0.6941136818767482
S	5.413064961260079	4.316819894800218	13.88327572377266

S	2.965024652297645	2.364552707054905	13.88327572377266
Mo	5.057319414049724	1.7696897181940607	14.230369050199387
S	3.004008480605437	6.237959548395224	11.80077489787687
S	1.6454558119016012	3.4168634541422183	11.80077489787687
Mo	3.7886498369139483	3.7887219174357374	12.147868224303597
S	-2.728900825823654e-05	6.923597784260712	9.718274071981078
S	-1.4947646629311864e-05	3.792424118285034	9.718274071981078
Mo	1.769593501340136	5.057353081842396	10.065367398407806
S	-3.004057653712199	6.237935867908365	7.635773246085288
S	-1.64548274663725	3.4168504830753976	7.635773246085288
Mo	-0.5999516860366892	5.324315855471739	7.982866572512016
S	-5.413098990143673	4.316777224026054	5.553272420189498
S	-2.9650432917338	2.3645293339939433	5.553272420189498
Mo	-2.8506693701383075	4.536735114216091	5.900365746616225
S	-6.750012265348259	1.540629967452474	3.4707715942937067
S	-3.697342062824629	0.8438852787204945	3.4707715942937067
Mo	-4.53677838357452	2.8506005073908525	3.8178649207204343
S	-6.750006046473266	-1.5406572141585826	1.3882707683979154
S	-3.697338656414805	-0.8439002031959781	1.3882707683979154
Mo	-5.324324961434673	0.5998708689790546	1.7353640948246434
S	-0.7752297867608297	6.880059960253494	12.842025310824766
S	-0.4246347393559144	3.768576127837354	12.842025310824766
Mo	1.1922184750913623	5.223686099112086	13.189118637251493
S	-3.683600823004167	5.862362258998292	10.759524484928974
S	-2.0177048174365124	3.2111287677181273	10.759524484928974
Mo	-1.1923178565693688	5.223663415966983	11.1066178113557
S	-5.862391296266445	3.68355461048482	8.677023659033184
S	-3.2111446729800304	2.0176795043726403	8.677023659033184
Mo	-3.340701582438571	4.189032620008879	9.024116985459912
S	-6.88006607109722	0.7751755519244686	6.594522833137393
S	-3.7685794750726864	0.4246050320407474	6.594522833137393
Mo	-4.827419981802745	2.324714535958686	6.94161615956412
S	-6.535062662626827	-2.286736161979624	4.512022007241602
S	-3.5796026904668534	-1.252567471865653	4.512022007241602
Mo	-5.358010951160183	-4.066422065230801e-05	4.859115333668329
S	-4.895713062587459	-4.895732824386464	2.4295211813458106
S	-2.6816433988939865	-2.6816542234862717	2.4295211813458106
Mo	-4.827384694754798	-2.324787810371766	2.776614507725386
S	-2.286709782895776	-6.535071893083755	0.3470203554500202
S	-1.252553022633199	-3.5796077464808747	0.3470203554500202
Mo	-3.340637997358466	-4.189083327532509	0.6941136818767468
S	-4.316819894800216	5.41306496126008	13.883275723772663
S	-2.3645527070549037	2.965024652297646	13.883275723772663
Mo	-1.7696897181940634	5.057319414049724	14.23036905019939
S	-6.237959548395224	3.004008480605437	11.80077489787687
S	-3.4168634541422183	1.6454558119016014	11.80077489787687
Mo	-3.7887219174357383	3.7886498369139483	12.147868224303599
S	-6.923597784260712	-2.728900825781259e-05	9.71827407198108

S	-3.792424118285034	-1.4947646629079643e-05	9.71827407198108
Mo	-5.057353081842396	1.7695935013401363	10.065367398407808
S	-6.237935867908367	-3.004057653712196	7.635773246085289
S	-3.4168504830753985	-1.6454827466372481	7.635773246085289
Mo	-5.324315855471739	-0.5999516860366854	7.982866572512016
S	-4.316777224026055	-5.413098990143673	5.553272420189499
S	-2.3645293339939437	-2.9650432917338	5.553272420189499
Mo	-4.536735114216091	-2.8506693701383066	5.900365746616226
S	-1.5406299674524744	-6.750012265348259	3.4707715942937067
S	-0.8438852787204947	-3.697342062824629	3.4707715942937067
Mo	-2.8506005073908547	-4.536778383574518	3.8178649207204347
S	1.540657214158579	-6.750006046473267	1.3882707683979172
S	0.8439002031959763	-3.6973386564148054	1.3882707683979172
Mo	-0.5998708689790574	-5.324324961434673	1.7353640948246438
S	-6.880059960253494	-0.7752297867608262	12.842025310824766
S	-3.768576127837354	-0.4246347393559125	12.842025310824766
Mo	-5.2236860991120855	1.192218475091366	13.189118637251493
S	-5.862362258998296	-3.6836008230041615	10.759524484928976
S	-3.211128767718129	-2.0177048174365093	10.759524484928976
Mo	-5.223663415966984	-1.1923178565693626	11.106617811355703
S	-3.683554610484823	-5.862391296266443	8.677023659033184
S	-2.017679504372642	-3.2111446729800295	8.677023659033184
Mo	-4.189032620008881	-3.340701582438569	9.024116985459912
S	-0.7751755519244721	-6.880066071097219	6.594522833137394
S	-0.4246050320407493	-3.768579475072686	6.594522833137394
Mo	-2.3247145359586905	-4.827419981802742	6.941616159564121
S	2.286736161979623	-6.535062662626827	4.512022007241603
S	1.2525674718656525	-3.5796026904668534	4.512022007241603
Mo	4.0664220651979926e-05	-5.358010951160183	4.8591153336683295
S	4.895732824386458	-4.895713062587465	2.4295211813458115
S	2.681654223486269	-2.6816433988939887	2.4295211813458115
Mo	2.3247878103717614	-4.8273846947548	2.776614507772539
S	6.535071893083753	-2.286709782895782	0.34702035545002197
S	3.5796077464808738	-1.2525530226332022	0.34702035545002197
Mo	4.189083327532505	-3.34063799735847	0.6941136818767486
S	-5.41306496126008	-4.316819894800216	13.883275723772663
S	-2.965024652297646	-2.3645527070549037	13.883275723772663
Mo	-5.057319414049725	-1.7696897181940585	14.23036905019939
S	-3.00400848060544	-6.237959548395223	11.800774897876872
S	-1.6454558119016032	-3.4168634541422174	11.800774897876872
Mo	-3.788649836913952	-3.7887219174357347	12.147868224303599
S	2.7289008251239257e-05	-6.923597784260712	9.71827407198108
S	1.4947646625479076e-05	-3.792424118285034	9.71827407198108
Mo	-1.7695935013401414	-5.057353081842394	10.065367398407808
S	3.004057653712198	-6.237935867908366	7.63577324608529
S	1.6454827466372495	-3.416850483075398	7.63577324608529
Mo	0.5999516860366874	-5.324315855471739	7.982866572512018
S	5.413098990143668	-4.316777224026059	5.553272420189499

S	2.965043291733797	-2.364529333993946	5.553272420189499
Mo	2.8506693701383004	-4.536735114216095	5.900365746616226
S	6.750012265348257	-1.540629967452481	3.4707715942937094
S	3.697342062824628	-0.8438852787204982	3.4707715942937094
Mo	4.536778383574518	-2.850600507390855	3.817864920720435
Mo	5.324324961434673	-0.5998708689790576	1.7353640948246447
S	0.7752297867608197	-6.880059960253494	12.842025310824766
S	0.4246347393559089	-3.7685761278373544	12.842025310824766
Mo	-1.192218475091371	-5.223686099112085	13.189118637251495
S	3.6836008230041584	-5.8623622589982975	10.759524484928976
S	2.017704817436508	-3.2111287677181304	10.759524484928976
Mo	1.1923178565693602	-5.223663415966985	11.106617811355704
S	5.862391296266442	-3.683554610484823	8.677023659033186
S	3.211144672980029	-2.017679504372642	8.677023659033186
Mo	3.3407015824385686	-4.189032620008881	9.024116985459912
S	6.880066071097218	-0.7751755519244786	6.594522833137395
S	3.7685794750726855	-0.42460503204075284	6.594522833137395
Mo	4.827419981802742	-2.324714535958691	6.941616159564122
S	4.3168198948002106	-5.413064961260084	13.883275723772663
S	2.3645527070549006	-2.965024652297648	13.883275723772663
Mo	1.7696897181940536	-5.057319414049727	14.23036905019939
S	6.237959548395217	-3.0040084806054517	11.800774897876872
S	3.4168634541422143	-1.6454558119016094	11.800774897876872
Mo	3.7887219174357276	-3.7886498369139585	12.147868224303599
Mo	5.057353081842394	-1.7695935013401416	10.065367398407808
Mo	5.223686099112085	-1.1922184750913714	13.189118637251495

alat

1.0

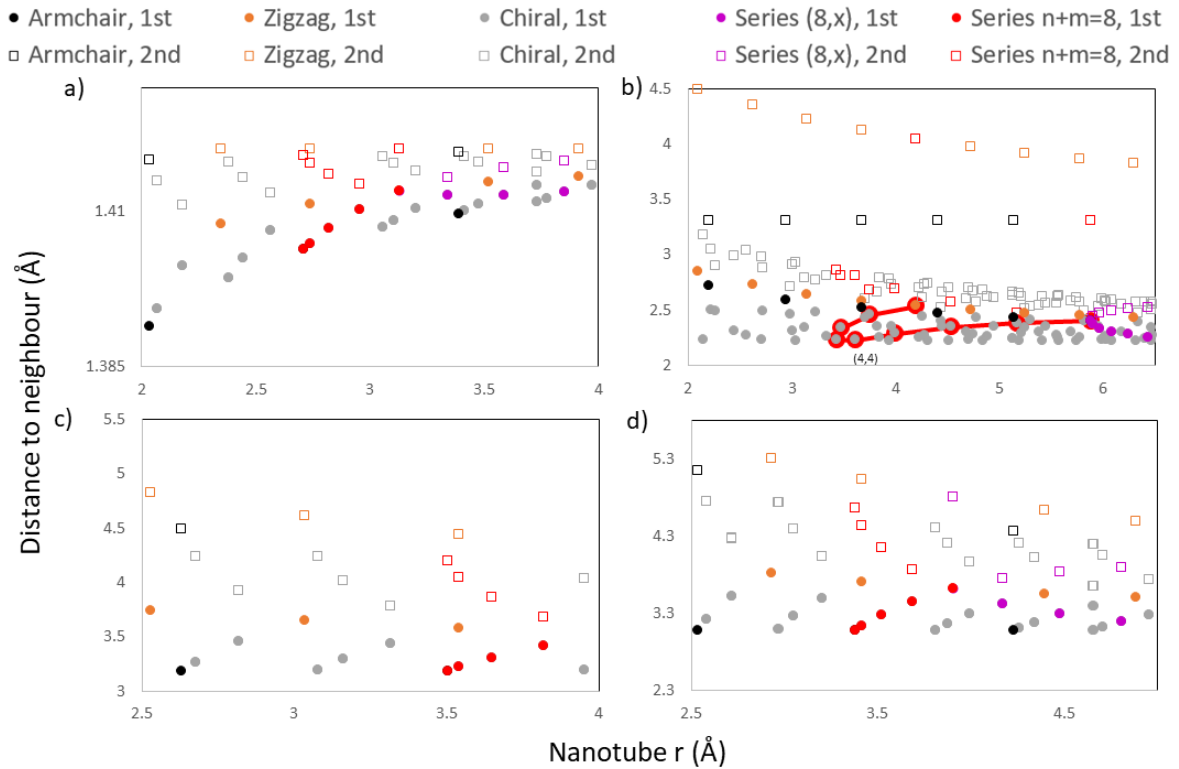
supercell

10.716021902628983 0.0 0.0

0.0 10.716021902628983 0.0

0.0 0.0 14.577505781285105

cartesian coordinates



Supplementary Figure 1: Zoom of plots in figure 6 from main paper. Plots of 1st and 2nd neighbours of the outermost atomic layer for all the chiral and achiral nanotubes in a small radius region including the series $n + m = 8$ for 4 different materials: **a)** SWCNTs, **b)** PNTs, **c)** MoS₂ NTs and **d)** Ti₃C₂ NTs. In the case of PNTs, the families of $(n, m) = X$ (with a fixed X), present a double trend that encounter at the point for the NT $(X/2, X/2) = X$ as exemplified with the red line in the series $m + n = 8$, which two branches encounter at the value for (4, 4).