Supplemental Information for

Stabilization of $NbTe_3$, VTe_3, and $TiTe_3$ *via* Nanotube Encapsulation

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Electron Microscopy Details:

After synthesis, filled CNT are cast onto TEM grids (Cu grid, 300 mesh, Lacey Carbon) for characterization. Initial imaging for confirmation and analysis of filling characteristics is done on a JEOL 2010 microscope (TEM, 80 kV). Elemental analysis is done on an aberration-corrected FEI Titan3 (60−300) equipped with a SuperX energy dispersive X-ray spectrometer (EDS, 80 kV, of the few-chain TMT limit). The spectral maps were summed vertically (along the

wire direction) to improve the signal to noise in the line scans presented in Figure2. Mapping thus served to distribute the dose over the sample reducing damage. Atomic-resolution STEM imaging for identification of the few chains and TAP single chains is completed at the National Center for Electron Microscopy on TEAM 0.5 which is a Titan 80-300 with a ultra-twin pole piece gap, DCOR probe aberration corrector and was operated at 80 kV and semi-convergence angle of 30 mrad. Images were acquired using the ADF-STEM detector with an inner angle of 60 mrad and a beam current of approximately 70 pA.

STEM simulations were done using EJ Kirkland's autostem program with parameters that matched the experiments. In detail for each simulation, we used a 15.0x30.0 Å square simulation box, 80 kV accelerating voltage, 30 mrad convergence semi-angle, 256 pixel sampling, 1 Å slice size, 0.13 Å STEM probe step size, and 50 frozen phonon calculations. After completion, the multislice data was convolved with a 1.1 Å source size to match the resolution and contrast seen in the experimental images. Noise was added following Poisson counting statistics to match the 70 pA experimental beam current. This allowed us to interpret the positions of atoms based on the approximate Z-contrast in the images and to compare the projection images to the DFT simulated structures.

Computational Methods:

We use the generalized gradient approximation,[1] norm-conserving pseudopotentials,[2] and localized pseudo-atomic orbitals for the wavefunction expansion as implemented in the SIESTA code.[3] The spin–orbit interaction is considered using fully relativistic j-dependent pseudopotentials[4] in the l-dependent fully-separable nonlocal form using additional Kleinman-Bylander-type projectors.[5] We use 1×1×128 Monkhorst-Pack *k*-point mesh for single chains, and

about 32 mesh per $Å^{-1}$ of the reciprocal vector for bulk materials. Real-space mesh cut-off of 500 Ry is used for all of our calculations. The van der Waals interaction is evaluated using the DFT-D2 correction.[6] Dipole corrections are included to reduce the fictitious interactions between chains generated by the periodic boundary condition in our supercell approach.[7] The crystallographic data for the TP and TAP single chains of $NbTe_3$, VTe_3, and $TiTe_3$ can be found in the tables below for both the encpsulated species and the species in vacuum.

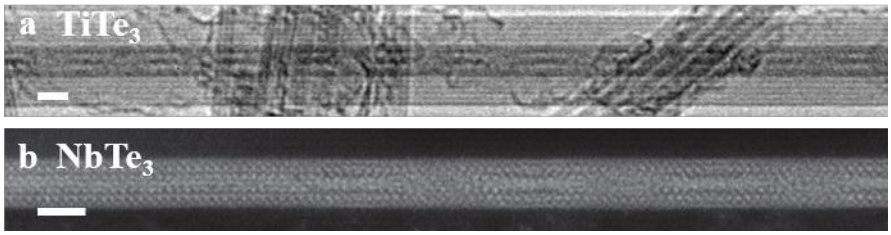

Figure S1. Tell-tale spiraling of the few-chain limit. (a) TEM image of few-chain twisting of $TiTe_3$ encapsulated within a MWCNT. (b) STEM image of few-chain twisting of $NbTe_3$ encapsulated within a MWCNT. Scale bars measure 2 nm.

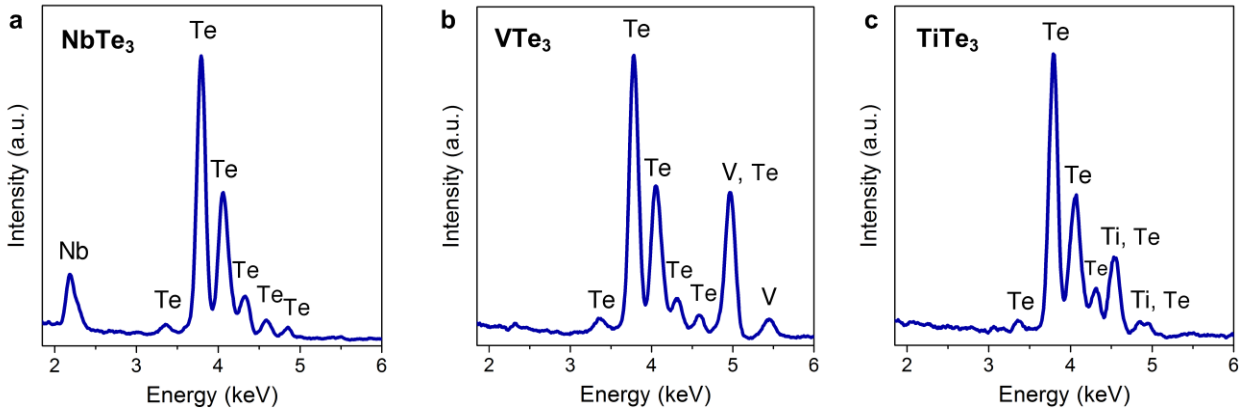

Figure S2. Energy Dispersive Spectroscopy Spectra. EDS spectra collected on few-chain specimen for (a) $NbTe_3$, (b) VTe_3, and (c) $TiTe_3$, with relevant peaks labeled.

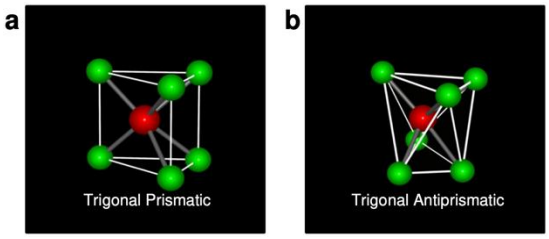

Figure S3. The geometry of the TP and TAP unit cell. The basic units of (a) the TP and (b) TAP geometry are shown for comparison.

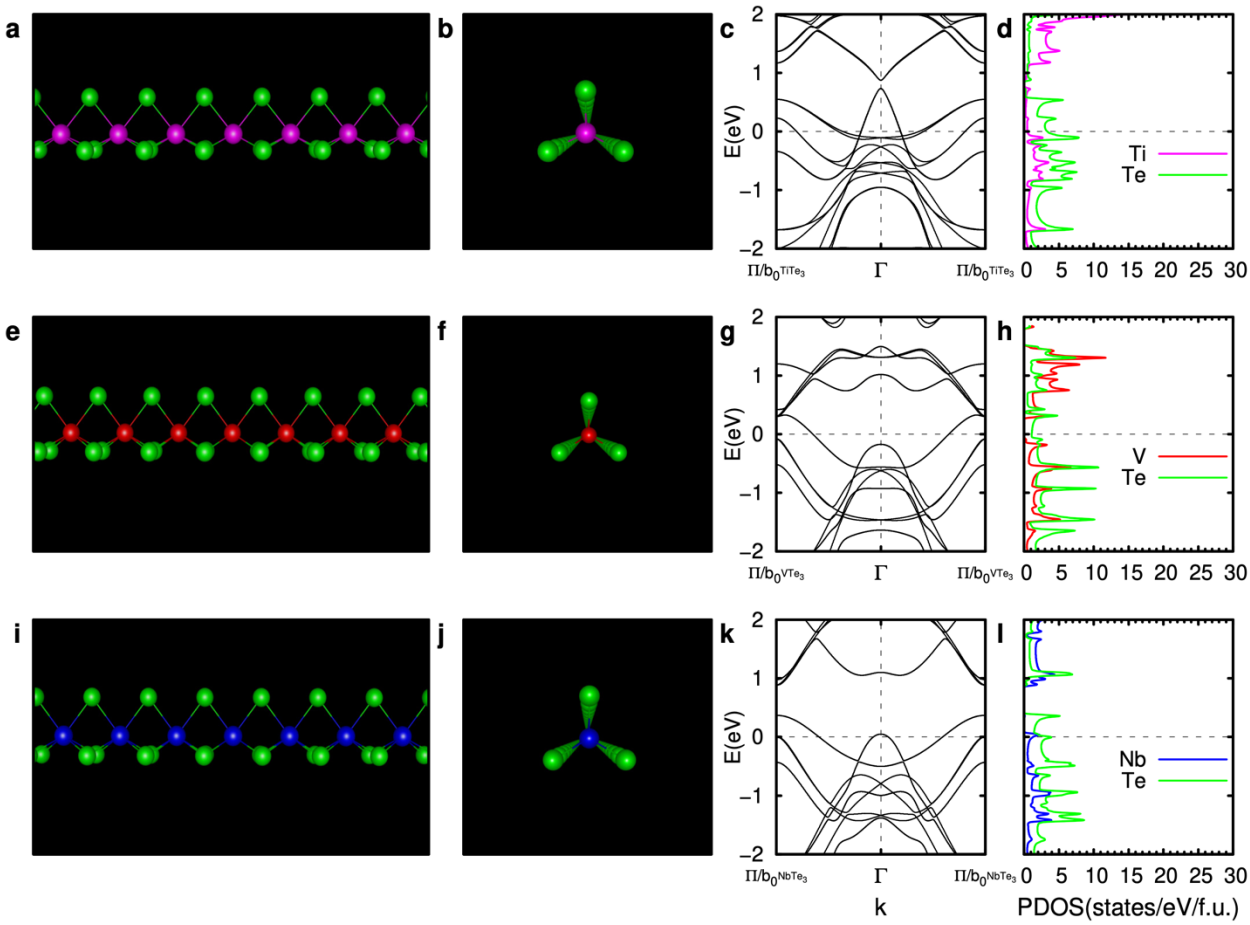

Figure S4. Calculated atomic structure and electronic structures for TP single-chain MTe_3 (M=Ti, V, and Nb) isolated in vacuum. (a-d) $TiTe_3$, (e-h) VTe_3, and (i-l) $NbTe_3$. In the 1st and 2nd columns, TP single-chain isolated in vacuum are presented side-on and end-on, respectively.

In the atomic structure, the magenta, red, blue, and green spheres represent the Ti, V, Nb, and Te atoms, respectively. In the band structures, the chemical potential is set to zero and marked with a horizontal dashed line, and the zone boundaries for the chains are denoted as π/b_0^{MTe3}, where b_0^{MTe3} is the distance between the nearest transition metal atoms. In d, h, and l, the density of states projected onto Ti, V, Nb, and Te atoms are presented by magenta, red, blue and green lines, respectively.

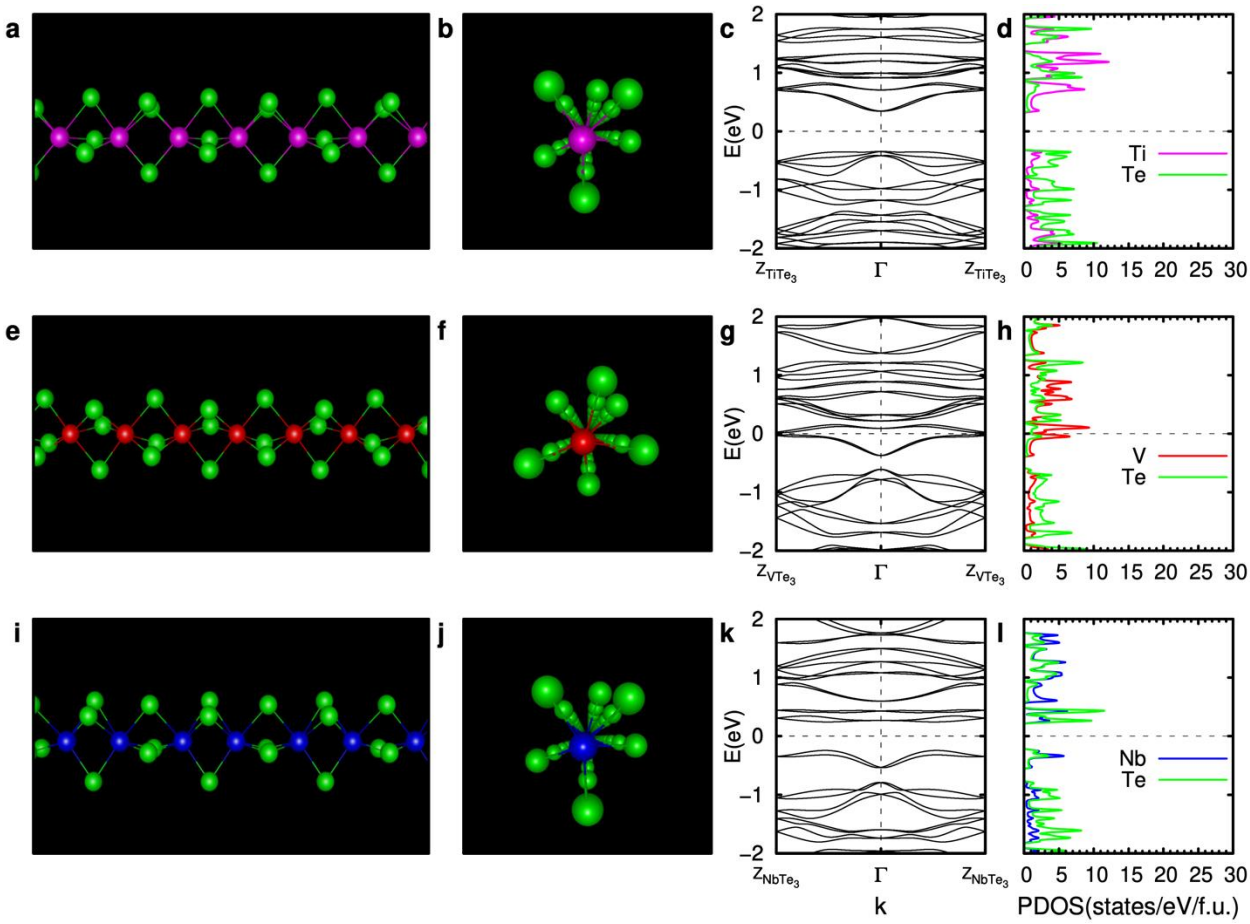

Figure S5. Calculated atomic structure and electronic structures for TAP single-chain MTe_3 (M=Ti, V, and Nb) isolated in vacuum. (a-d) $TiTe_3$, (e-h) VTe_3, and (i-l) $NbTe_3$. In the 1st and 2nd columns, TAP single-chain encapsulated isolated in vacuum are presented side-on and

end-on, respectively. In the atomic structure, the magenta, red, blue, and green spheres represent the Ti, V, Nb, and Te atoms, respectively. In the band structures, the chemical potential is set to zero and marked with a horizontal dashed line, and the zone boundaries for the chains are denoted as Z_{MTe3}. Here, the lengths of the first Brillouin zones of the TAP chains are half of those in the corresponding TP chains because of the doubled real-space unit cell length of the rocking chains, i.e. $Z_{MTe3} = \pi/2\ b_0^{MTe3}$ where b_0^{MTe3} is the distance between the nearest transition metal atoms. In d, h, and l, the density of states projected onto Ti, V, Nb, and Te atoms are presented by magenta, red, blue and green lines, respectively.

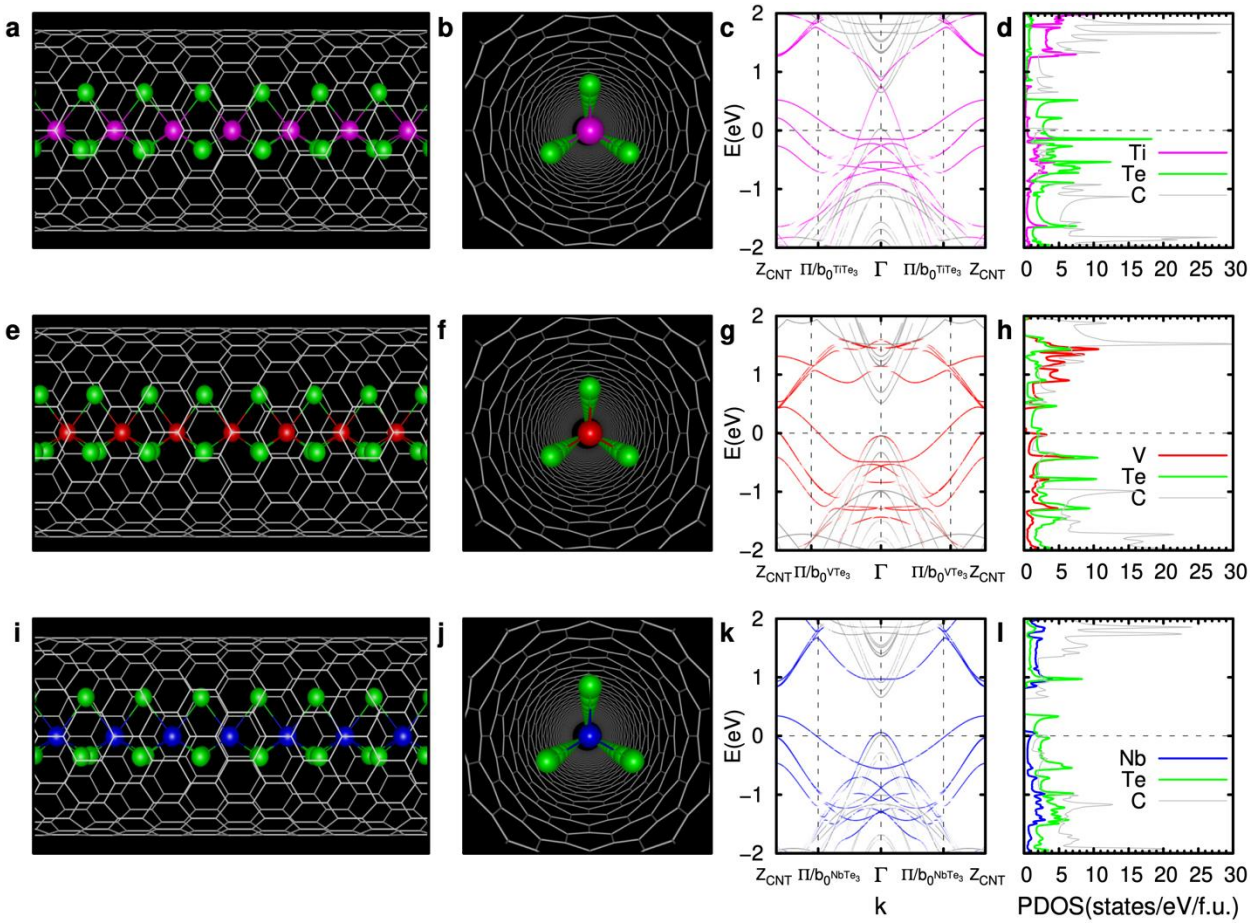

Figure S6. Calculated atomic structure and electronic structures for TP single-chain MTe_3 (M=Ti, V, and Nb) encapsulated in CNT. (a-d) $TiTe_3$, (e-h) VTe_3, and (i-l) $NbTe_3$. In the 1st and 2nd columns, TP single-chain encapsulated inside a (14,0) CNT are presented side-on and end-on, respectively. In the atomic structure, the magenta, red, blue, and green spheres represent the Ti, V, Nb, and Te atoms, respectively. In the band structures, the chemical potential is set to zero and marked with a horizontal dashed line. In c, g, and k, the bands represented by magenta, red, blue and gray lines are projected onto the single-chain $TiTe_3$, VTe_3, $NbTe_3$ and CNT, respectively. The bands are then unfolded with respect to the first Brillouin zone of the unit cell of the single chain and the CNT, where zone boundaries for the chain and CNT are denoted as π/b_0^{MTe3} and Z_{CNT}, respectively, and b_0^{MTe3} is the distance between the nearest transition metal atoms. In d, h, and l, the density of states projected onto Ti, V, Nb, Te, and C atoms are presented by magenta, red, blue, green, and gray lines, respectively.

REFERENCES

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Crystallography Data

Table S1. Calculated atomic positions for TAP single-chain $TiTe_3$ encapsulated in a CNT.

The lengths of the lattice vectors are 15 Å, 15 Å, and 21.84 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	Ti	7.394190	7.330035	0.910138
2	Te	9.592755	7.198440	2.731922
3	Te	8.053575	9.529620	2.735023
4	Te	5.606190	6.517995	2.730349
5	Ti	7.394490	7.324425	4.548988
6	Te	9.035460	8.929845	6.367605
7	Te	6.255225	9.204510	6.369920
8	Te	7.505685	5.369265	6.369287
9	Ti	7.397085	7.324320	8.190939
10	Te	9.595830	7.174695	10.008464
11	Te	8.081190	9.517860	10.008049
12	Te	5.602860	6.525390	10.009818
13	Ti	7.397310	7.327890	11.829221
14	Te	9.040500	8.927145	13.654062
15	Te	6.262575	9.214575	13.651922
16	Te	7.501650	5.369145	13.650655
17	Ti	7.392570	7.326000	15.470713
18	Te	9.588135	7.191675	17.289614
19	Te	8.056560	9.527280	17.286906
20	Te	5.605635	6.518565	17.289527
21	Ti	7.391925	7.328130	19.109541
22	Te	9.020340	8.945760	20.927634
23	Te	6.240270	9.205680	20.928398
24	Te	7.513110	5.369280	20.929840
25	C	13.130955	7.500000	0.364007
26	C	13.130955	7.500000	1.819993
27	C	12.989775	8.753010	2.548007
28	C	12.989775	8.753010	4.003993
29	C	12.573315	9.943185	0.364007
30	C	12.573315	9.943185	1.819993
31	C	11.902455	11.010840	2.548007

32	C	11.902455	11.010840	4.003993
33	C	11.010840	11.902455	0.364007
34	C	11.010840	11.902455	1.819993
35	C	9.943185	12.573315	2.548007
36	C	9.943185	12.573315	4.003993
37	C	8.753010	12.989775	0.364007
38	C	8.753010	12.989775	1.819993
39	C	7.500000	13.130955	2.548007
40	C	7.500000	13.130955	4.003993
41	C	6.246990	12.989775	0.364007
42	C	6.246990	12.989775	1.819993
43	C	5.056815	12.573315	2.548007
44	C	5.056815	12.573315	4.003993
45	C	3.989160	11.902455	0.364007
46	C	3.989160	11.902455	1.819993
47	C	3.097545	11.010840	2.548007
48	C	3.097545	11.010840	4.003993
49	C	2.426685	9.943185	0.364007
50	C	2.426685	9.943185	1.819993
51	C	2.010225	8.753010	2.548007
52	C	2.010225	8.753010	4.003993
53	C	1.869045	7.500000	0.364007
54	C	1.869045	7.500000	1.819993
55	C	2.010225	6.246990	2.548007
56	C	2.010225	6.246990	4.003993
57	C	2.426685	5.056815	0.364007
58	C	2.426685	5.056815	1.819993
59	C	3.097545	3.989160	2.548007
60	C	3.097545	3.989160	4.003993
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62	C	3.989160	3.097545	1.819993
63	C	5.056815	2.426685	2.548007
64	C	5.056815	2.426685	4.003993
65	C	6.246990	2.010225	0.364007
66	C	6.246990	2.010225	1.819993
67	C	7.500000	1.869045	2.548007
68	C	7.500000	1.869045	4.003993
69	C	8.753010	2.010225	0.364007
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83	C	12.989775	8.753010	6.916007
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210	C	6.246990	12.989775	14.923993
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217	C	2.426685	9.943185	13.468007
218	C	2.426685	9.943185	14.923993
219	C	2.010225	8.753010	15.652007
220	C	2.010225	8.753010	17.107993
221	C	1.869045	7.500000	13.468007
222	C	1.869045	7.500000	14.923993
223	C	2.010225	6.246990	15.652007
224	C	2.010225	6.246990	17.107993
225	C	2.426685	5.056815	13.468007
226	C	2.426685	5.056815	14.923993

227	C	3.097545	3.989160	15.652007
228	C	3.097545	3.989160	17.107993
229	C	3.989160	3.097545	13.468007
230	C	3.989160	3.097545	14.923993
231	C	5.056815	2.426685	15.652007
232	C	5.056815	2.426685	17.107993
233	C	6.246990	2.010225	13.468007
234	C	6.246990	2.010225	14.923993
235	C	7.500000	1.869045	15.652007
236	C	7.500000	1.869045	17.107993
237	C	8.753010	2.010225	13.468007
238	C	8.753010	2.010225	14.923993
239	C	9.943185	2.426685	15.652007
240	C	9.943185	2.426685	17.107993
241	C	11.010840	3.097545	13.468007
242	C	11.010840	3.097545	14.923993
243	C	11.902455	3.989160	15.652007
244	C	11.902455	3.989160	17.107993
245	C	12.573315	5.056815	13.468007
246	C	12.573315	5.056815	14.923993
247	C	12.989775	6.246990	15.652007
248	C	12.989775	6.246990	17.107993
249	C	13.130955	7.500000	17.836007
250	C	13.130955	7.500000	19.291993
251	C	12.989775	8.753010	20.020007
252	C	12.989775	8.753010	21.475993
253	C	12.573315	9.943185	17.836007
254	C	12.573315	9.943185	19.291993
255	C	11.902455	11.010840	20.020007
256	C	11.902455	11.010840	21.475993
257	C	11.010840	11.902455	17.836007
258	C	11.010840	11.902455	19.291993
259	C	9.943185	12.573315	20.020007
260	C	9.943185	12.573315	21.475993
261	C	8.753010	12.989775	17.836007
262	C	8.753010	12.989775	19.291993
263	C	7.500000	13.130955	20.020007
264	C	7.500000	13.130955	21.475993
265	C	6.246990	12.989775	17.836007

266	C	6.246990	12.989775	19.291993
267	C	5.056815	12.573315	20.020007
268	C	5.056815	12.573315	21.475993
269	C	3.989160	11.902455	17.836007
270	C	3.989160	11.902455	19.291993
271	C	3.097545	11.010840	20.020007
272	C	3.097545	11.010840	21.475993
273	C	2.426685	9.943185	17.836007
274	C	2.426685	9.943185	19.291993
275	C	2.010225	8.753010	20.020007
276	C	2.010225	8.753010	21.475993
277	C	1.869045	7.500000	17.836007
278	C	1.869045	7.500000	19.291993
279	C	2.010225	6.246990	20.020007
280	C	2.010225	6.246990	21.475993
281	C	2.426685	5.056815	17.836007
282	C	2.426685	5.056815	19.291993
283	C	3.097545	3.989160	20.020007
284	C	3.097545	3.989160	21.475993
285	C	3.989160	3.097545	17.836007
286	C	3.989160	3.097545	19.291993
287	C	5.056815	2.426685	20.020007
288	C	5.056815	2.426685	21.475993
289	C	6.246990	2.010225	17.836007
290	C	6.246990	2.010225	19.291993
291	C	7.500000	1.869045	20.020007
292	C	7.500000	1.869045	21.475993
293	C	8.753010	2.010225	17.836007
294	C	8.753010	2.010225	19.291993
295	C	9.943185	2.426685	20.020007
296	C	9.943185	2.426685	21.475993
297	C	11.010840	3.097545	17.836007
298	C	11.010840	3.097545	19.291993
299	C	11.902455	3.989160	20.020007
300	C	11.902455	3.989160	21.475993
301	C	12.573315	5.056815	17.836007
302	C	12.573315	5.056815	19.291993
303	C	12.989775	6.246990	20.020007
304	C	12.989775	6.246990	21.475993

Table S2. Calculated atomic positions for TAP single-chain VTe_3 encapsulated in a CNT. The lengths of the lattice vectors are 15 Å, 15 Å, and 13.62 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	V	7.414290	7.451610	0.403928
2	Te	9.033285	7.247715	2.163033
3	Te	7.961715	9.032280	2.163823
4	Te	6.036060	6.866610	2.161889
5	V	7.413540	7.448655	3.921348
6	Te	8.583705	8.689935	5.568986
7	Te	6.476070	8.804235	5.569409
8	Te	7.637685	5.920995	5.568796
9	V	7.412295	7.448145	7.215890
10	Te	9.033300	7.247370	8.973809
11	Te	7.960260	9.033120	8.971766
12	Te	6.035505	6.866400	8.974518
13	V	7.414110	7.451415	10.733473
14	Te	8.583225	8.693415	12.378714
15	Te	6.475650	8.804910	12.379313
16	Te	7.638030	5.922255	12.378809
17	C	11.889510	7.500000	0.378336
18	C	11.889510	7.500000	1.891668
19	C	11.779455	8.476755	2.648327
20	C	11.779455	8.476755	4.161673
21	C	11.454810	9.404535	0.378336
22	C	11.454810	9.404535	1.891668
23	C	10.931865	10.236810	2.648327
24	C	10.931865	10.236810	4.161673
25	C	10.236810	10.931865	0.378336
26	C	10.236810	10.931865	1.891668
27	C	9.404535	11.454810	2.648327
28	C	9.404535	11.454810	4.161673
29	C	8.476755	11.779455	0.378336
30	C	8.476755	11.779455	1.891668
31	C	7.500000	11.889510	2.648327
32	C	7.500000	11.889510	4.161673
33	C	6.523245	11.779455	0.378336

34	C	6.523245	11.779455	1.891668
35	C	5.595465	11.454810	2.648327
36	C	5.595465	11.454810	4.161673
37	C	4.763190	10.931865	0.378336
38	C	4.763190	10.931865	1.891668
39	C	4.068135	10.236810	2.648327
40	C	4.068135	10.236810	4.161673
41	C	3.545190	9.404535	0.378336
42	C	3.545190	9.404535	1.891668
43	C	3.220545	8.476755	2.648327
44	C	3.220545	8.476755	4.161673
45	C	3.110490	7.500000	0.378336
46	C	3.110490	7.500000	1.891668
47	C	3.220545	6.523245	2.648327
48	C	3.220545	6.523245	4.161673
49	C	3.545190	5.595465	0.378336
50	C	3.545190	5.595465	1.891668
51	C	4.068135	4.763190	2.648327
52	C	4.068135	4.763190	4.161673
53	C	4.763190	4.068135	0.378336
54	C	4.763190	4.068135	1.891668
55	C	5.595465	3.545190	2.648327
56	C	5.595465	3.545190	4.161673
57	C	6.523245	3.220545	0.378336
58	C	6.523245	3.220545	1.891668
59	C	7.500000	3.110490	2.648327
60	C	7.500000	3.110490	4.161673
61	C	8.476755	3.220545	0.378336
62	C	8.476755	3.220545	1.891668
63	C	9.404535	3.545190	2.648327
64	C	9.404535	3.545190	4.161673
65	C	10.236810	4.068135	0.378336
66	C	10.236810	4.068135	1.891668
67	C	10.931865	4.763190	2.648327
68	C	10.931865	4.763190	4.161673
69	C	11.454810	5.595465	0.378336
70	C	11.454810	5.595465	1.891668
71	C	11.779455	6.523245	2.648327
72	C	11.779455	6.523245	4.161673

73	C	11.889510	7.500000	4.918332
74	C	11.889510	7.500000	6.431664
75	C	11.779455	8.476755	7.188336
76	C	11.779455	8.476755	8.701668
77	C	11.454810	9.404535	4.918332
78	C	11.454810	9.404535	6.431664
79	C	10.931865	10.236810	7.188336
80	C	10.931865	10.236810	8.701668
81	C	10.236810	10.931865	4.918332
82	C	10.236810	10.931865	6.431664
83	C	9.404535	11.454810	7.188336
84	C	9.404535	11.454810	8.701668
85	C	8.476755	11.779455	4.918332
86	C	8.476755	11.779455	6.431664
87	C	7.500000	11.889510	7.188336
88	C	7.500000	11.889510	8.701668
89	C	6.523245	11.779455	4.918332
90	C	6.523245	11.779455	6.431664
91	C	5.595465	11.454810	7.188336
92	C	5.595465	11.454810	8.701668
93	C	4.763190	10.931865	4.918332
94	C	4.763190	10.931865	6.431664
95	C	4.068135	10.236810	7.188336
96	C	4.068135	10.236810	8.701668
97	C	3.545190	9.404535	4.918332
98	C	3.545190	9.404535	6.431664
99	C	3.220545	8.476755	7.188336
100	C	3.220545	8.476755	8.701668
101	C	3.110490	7.500000	4.918332
102	C	3.110490	7.500000	6.431664
103	C	3.220545	6.523245	7.188336
104	C	3.220545	6.523245	8.701668
105	C	3.545190	5.595465	4.918332
106	C	3.545190	5.595465	6.431664
107	C	4.068135	4.763190	7.188336
108	C	4.068135	4.763190	8.701668
109	C	4.763190	4.068135	4.918332
110	C	4.763190	4.068135	6.431664
111	C	5.595465	3.545190	7.188336

112	C	5.595465	3.545190	8.701668
113	C	6.523245	3.220545	4.918332
114	C	6.523245	3.220545	6.431664
115	C	7.500000	3.110490	7.188336
116	C	7.500000	3.110490	8.701668
117	C	8.476755	3.220545	4.918332
118	C	8.476755	3.220545	6.431664
119	C	9.404535	3.545190	7.188336
120	C	9.404535	3.545190	8.701668
121	C	10.236810	4.068135	4.918332
122	C	10.236810	4.068135	6.431664
123	C	10.931865	4.763190	7.188336
124	C	10.931865	4.763190	8.701668
125	C	11.454810	5.595465	4.918332
126	C	11.454810	5.595465	6.431664
127	C	11.779455	6.523245	7.188336
128	C	11.779455	6.523245	8.701668
129	C	11.889510	7.500000	9.458327
130	C	11.889510	7.500000	10.971673
131	C	11.779455	8.476755	11.728332
132	C	11.779455	8.476755	13.241664
133	C	11.454810	9.404535	9.458327
134	C	11.454810	9.404535	10.971673
135	C	10.931865	10.236810	11.728332
136	C	10.931865	10.236810	13.241664
137	C	10.236810	10.931865	9.458327
138	C	10.236810	10.931865	10.971673
139	C	9.404535	11.454810	11.728332
140	C	9.404535	11.454810	13.241664
141	C	8.476755	11.779455	9.458327
142	C	8.476755	11.779455	10.971673
143	C	7.500000	11.889510	11.728332
144	C	7.500000	11.889510	13.241664
145	C	6.523245	11.779455	9.458327
146	C	6.523245	11.779455	10.971673
147	C	5.595465	11.454810	11.728332
148	C	5.595465	11.454810	13.241664
149	C	4.763190	10.931865	9.458327
150	C	4.763190	10.931865	10.971673

151	C	4.068135	10.236810	11.728332
152	C	4.068135	10.236810	13.241664
153	C	3.545190	9.404535	9.458327
154	C	3.545190	9.404535	10.971673
155	C	3.220545	8.476755	11.728332
156	C	3.220545	8.476755	13.241664
157	C	3.110490	7.500000	9.458327
158	C	3.110490	7.500000	10.971673
159	C	3.220545	6.523245	11.728332
160	C	3.220545	6.523245	13.241664
161	C	3.545190	5.595465	9.458327
162	C	3.545190	5.595465	10.971673
163	C	4.068135	4.763190	11.728332
164	C	4.068135	4.763190	13.241664
165	C	4.763190	4.068135	9.458327
166	C	4.763190	4.068135	10.971673
167	C	5.595465	3.545190	11.728332
168	C	5.595465	3.545190	13.241664
169	C	6.523245	3.220545	9.458327
170	C	6.523245	3.220545	10.971673
171	C	7.500000	3.110490	11.728332
172	C	7.500000	3.110490	13.241664
173	C	8.476755	3.220545	9.458327
174	C	8.476755	3.220545	10.971673
175	C	9.404535	3.545190	11.728332
176	C	9.404535	3.545190	13.241664
177	C	10.236810	4.068135	9.458327
178	C	10.236810	4.068135	10.971673
179	C	10.931865	4.763190	11.728332
180	C	10.931865	4.763190	13.241664
181	C	11.454810	5.595465	9.458327
182	C	11.454810	5.595465	10.971673
183	C	11.779455	6.523245	11.728332
184	C	11.779455	6.523245	13.241664

Table S3. Calculated atomic positions for TAP single-chain $NbTe_3$ encapsulated in a CNT. The lengths of the lattice vectors are 15 Å, 15 Å, and 21.48 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	Nb	7.438020	7.311885	0.586275
2	Te	9.740355	7.285530	2.256517
3	Te	8.113725	9.607785	2.257741
4	Te	5.352240	6.700830	2.256517
5	Nb	7.437930	7.309260	3.923043
6	Te	9.020610	8.989515	5.831799
7	Te	6.242190	9.198360	5.829285
8	Te	7.633170	5.292930	5.832486
9	Nb	7.439025	7.314975	7.746118
10	Te	9.739545	7.278330	9.418980
11	Te	8.121570	9.605820	9.419302
12	Te	5.347305	6.709620	9.418787
13	Nb	7.438365	7.307985	11.082327
14	Te	9.014100	8.996130	12.996689
15	Te	6.231345	9.182160	12.995250
16	Te	7.636020	5.293185	12.995593
17	Nb	7.438860	7.304745	14.907743
18	Te	9.740580	7.301370	16.569844
19	Te	8.087265	9.611100	16.567631
20	Te	5.353485	6.692340	16.569543
21	Nb	7.439400	7.313880	18.245477
22	Te	9.006375	9.003900	20.156467
23	Te	6.224880	9.187485	20.160333
24	Te	7.645230	5.292945	20.157691
25	C	13.038135	7.500000	0.358007
26	C	13.038135	7.500000	1.789993
27	C	12.899280	8.732355	2.506007
28	C	12.899280	8.732355	3.937993
29	C	12.489690	9.902910	0.358007
30	C	12.489690	9.902910	1.789993
31	C	11.829885	10.952970	2.506007
32	C	11.829885	10.952970	3.937993
33	C	10.952970	11.829885	0.358007

34	C	10.952970	11.829885	1.789993
35	C	9.902910	12.489690	2.506007
36	C	9.902910	12.489690	3.937993
37	C	8.732355	12.899280	0.358007
38	C	8.732355	12.899280	1.789993
39	C	7.500000	13.038135	2.506007
40	C	7.500000	13.038135	3.937993
41	C	6.267645	12.899280	0.358007
42	C	6.267645	12.899280	1.789993
43	C	5.097090	12.489690	2.506007
44	C	5.097090	12.489690	3.937993
45	C	4.047030	11.829885	0.358007
46	C	4.047030	11.829885	1.789993
47	C	3.170115	10.952970	2.506007
48	C	3.170115	10.952970	3.937993
49	C	2.510310	9.902910	0.358007
50	C	2.510310	9.902910	1.789993
51	C	2.100720	8.732355	2.506007
52	C	2.100720	8.732355	3.937993
53	C	1.961865	7.500000	0.358007
54	C	1.961865	7.500000	1.789993
55	C	2.100720	6.267645	2.506007
56	C	2.100720	6.267645	3.937993
57	C	2.510310	5.097090	0.358007
58	C	2.510310	5.097090	1.789993
59	C	3.170115	4.047030	2.506007
60	C	3.170115	4.047030	3.937993
61	C	4.047030	3.170115	0.358007
62	C	4.047030	3.170115	1.789993
63	C	5.097090	2.510310	2.506007
64	C	5.097090	2.510310	3.937993
65	C	6.267645	2.100720	0.358007
66	C	6.267645	2.100720	1.789993
67	C	7.500000	1.961865	2.506007
68	C	7.500000	1.961865	3.937993
69	C	8.732355	2.100720	0.358007
70	C	8.732355	2.100720	1.789993
71	C	9.902910	2.510310	2.506007
72	C	9.902910	2.510310	3.937993

73	C	10.952970	3.170115	0.358007
74	C	10.952970	3.170115	1.789993
75	C	11.829885	4.047030	2.506007
76	C	11.829885	4.047030	3.937993
77	C	12.489690	5.097090	0.358007
78	C	12.489690	5.097090	1.789993
79	C	12.899280	6.267645	2.506007
80	C	12.899280	6.267645	3.937993
81	C	13.038135	7.500000	4.654007
82	C	13.038135	7.500000	6.085993
83	C	12.899280	8.732355	6.802007
84	C	12.899280	8.732355	8.233993
85	C	12.489690	9.902910	4.654007
86	C	12.489690	9.902910	6.085993
87	C	11.829885	10.952970	6.802007
88	C	11.829885	10.952970	8.233993
89	C	10.952970	11.829885	4.654007
90	C	10.952970	11.829885	6.085993
91	C	9.902910	12.489690	6.802007
92	C	9.902910	12.489690	8.233993
93	C	8.732355	12.899280	4.654007
94	C	8.732355	12.899280	6.085993
95	C	7.500000	13.038135	6.802007
96	C	7.500000	13.038135	8.233993
97	C	6.267645	12.899280	4.654007
98	C	6.267645	12.899280	6.085993
99	C	5.097090	12.489690	6.802007
100	C	5.097090	12.489690	8.233993
101	C	4.047030	11.829885	4.654007
102	C	4.047030	11.829885	6.085993
103	C	3.170115	10.952970	6.802007
104	C	3.170115	10.952970	8.233993
105	C	2.510310	9.902910	4.654007
106	C	2.510310	9.902910	6.085993
107	C	2.100720	8.732355	6.802007
108	C	2.100720	8.732355	8.233993
109	C	1.961865	7.500000	4.654007
110	C	1.961865	7.500000	6.085993
111	C	2.100720	6.267645	6.802007

112	C	2.100720	6.267645	8.233993
113	C	2.510310	5.097090	4.654007
114	C	2.510310	5.097090	6.085993
115	C	3.170115	4.047030	6.802007
116	C	3.170115	4.047030	8.233993
117	C	4.047030	3.170115	4.654007
118	C	4.047030	3.170115	6.085993
119	C	5.097090	2.510310	6.802007
120	C	5.097090	2.510310	8.233993
121	C	6.267645	2.100720	4.654007
122	C	6.267645	2.100720	6.085993
123	C	7.500000	1.961865	6.802007
124	C	7.500000	1.961865	8.233993
125	C	8.732355	2.100720	4.654007
126	C	8.732355	2.100720	6.085993
127	C	9.902910	2.510310	6.802007
128	C	9.902910	2.510310	8.233993
129	C	10.952970	3.170115	4.654007
130	C	10.952970	3.170115	6.085993
131	C	11.829885	4.047030	6.802007
132	C	11.829885	4.047030	8.233993
133	C	12.489690	5.097090	4.654007
134	C	12.489690	5.097090	6.085993
135	C	12.899280	6.267645	6.802007
136	C	12.899280	6.267645	8.233993
137	C	13.038135	7.500000	8.950007
138	C	13.038135	7.500000	10.381993
139	C	12.899280	8.732355	11.098007
140	C	12.899280	8.732355	12.529993
141	C	12.489690	9.902910	8.950007
142	C	12.489690	9.902910	10.381993
143	C	11.829885	10.952970	11.098007
144	C	11.829885	10.952970	12.529993
145	C	10.952970	11.829885	8.950007
146	C	10.952970	11.829885	10.381993
147	C	9.902910	12.489690	11.098007
148	C	9.902910	12.489690	12.529993
149	C	8.732355	12.899280	8.950007
150	C	8.732355	12.899280	10.381993

151	C	7.500000	13.038135	11.098007
152	C	7.500000	13.038135	12.529993
153	C	6.267645	12.899280	8.950007
154	C	6.267645	12.899280	10.381993
155	C	5.097090	12.489690	11.098007
156	C	5.097090	12.489690	12.529993
157	C	4.047030	11.829885	8.950007
158	C	4.047030	11.829885	10.381993
159	C	3.170115	10.952970	11.098007
160	C	3.170115	10.952970	12.529993
161	C	2.510310	9.902910	8.950007
162	C	2.510310	9.902910	10.381993
163	C	2.100720	8.732355	11.098007
164	C	2.100720	8.732355	12.529993
165	C	1.961865	7.500000	8.950007
166	C	1.961865	7.500000	10.381993
167	C	2.100720	6.267645	11.098007
168	C	2.100720	6.267645	12.529993
169	C	2.510310	5.097090	8.950007
170	C	2.510310	5.097090	10.381993
171	C	3.170115	4.047030	11.098007
172	C	3.170115	4.047030	12.529993
173	C	4.047030	3.170115	8.950007
174	C	4.047030	3.170115	10.381993
175	C	5.097090	2.510310	11.098007
176	C	5.097090	2.510310	12.529993
177	C	6.267645	2.100720	8.950007
178	C	6.267645	2.100720	10.381993
179	C	7.500000	1.961865	11.098007
180	C	7.500000	1.961865	12.529993
181	C	8.732355	2.100720	8.950007
182	C	8.732355	2.100720	10.381993
183	C	9.902910	2.510310	11.098007
184	C	9.902910	2.510310	12.529993
185	C	10.952970	3.170115	8.950007
186	C	10.952970	3.170115	10.381993
187	C	11.829885	4.047030	11.098007
188	C	11.829885	4.047030	12.529993
189	C	12.489690	5.097090	8.950007

190	C	12.489690	5.097090	10.381993
191	C	12.899280	6.267645	11.098007
192	C	12.899280	6.267645	12.529993
193	C	13.038135	7.500000	13.246007
194	C	13.038135	7.500000	14.677993
195	C	12.899280	8.732355	15.394007
196	C	12.899280	8.732355	16.825993
197	C	12.489690	9.902910	13.246007
198	C	12.489690	9.902910	14.677993
199	C	11.829885	10.952970	15.394007
200	C	11.829885	10.952970	16.825993
201	C	10.952970	11.829885	13.246007
202	C	10.952970	11.829885	14.677993
203	C	9.902910	12.489690	15.394007
204	C	9.902910	12.489690	16.825993
205	C	8.732355	12.899280	13.246007
206	C	8.732355	12.899280	14.677993
207	C	7.500000	13.038135	15.394007
208	C	7.500000	13.038135	16.825993
209	C	6.267645	12.899280	13.246007
210	C	6.267645	12.899280	14.677993
211	C	5.097090	12.489690	15.394007
212	C	5.097090	12.489690	16.825993
213	C	4.047030	11.829885	13.246007
214	C	4.047030	11.829885	14.677993
215	C	3.170115	10.952970	15.394007
216	C	3.170115	10.952970	16.825993
217	C	2.510310	9.902910	13.246007
218	C	2.510310	9.902910	14.677993
219	C	2.100720	8.732355	15.394007
220	C	2.100720	8.732355	16.825993
221	C	1.961865	7.500000	13.246007
222	C	1.961865	7.500000	14.677993
223	C	2.100720	6.267645	15.394007
224	C	2.100720	6.267645	16.825993
225	C	2.510310	5.097090	13.246007
226	C	2.510310	5.097090	14.677993
227	C	3.170115	4.047030	15.394007
228	C	3.170115	4.047030	16.825993

229	C	4.047030	3.170115	13.246007
230	C	4.047030	3.170115	14.677993
231	C	5.097090	2.510310	15.394007
232	C	5.097090	2.510310	16.825993
233	C	6.267645	2.100720	13.246007
234	C	6.267645	2.100720	14.677993
235	C	7.500000	1.961865	15.394007
236	C	7.500000	1.961865	16.825993
237	C	8.732355	2.100720	13.246007
238	C	8.732355	2.100720	14.677993
239	C	9.902910	2.510310	15.394007
240	C	9.902910	2.510310	16.825993
241	C	10.952970	3.170115	13.246007
242	C	10.952970	3.170115	14.677993
243	C	11.829885	4.047030	15.394007
244	C	11.829885	4.047030	16.825993
245	C	12.489690	5.097090	13.246007
246	C	12.489690	5.097090	14.677993
247	C	12.899280	6.267645	15.394007
248	C	12.899280	6.267645	16.825993
249	C	13.038135	7.500000	17.542007
250	C	13.038135	7.500000	18.973993
251	C	12.899280	8.732355	19.690007
252	C	12.899280	8.732355	21.121993
253	C	12.489690	9.902910	17.542007
254	C	12.489690	9.902910	18.973993
255	C	11.829885	10.952970	19.690007
256	C	11.829885	10.952970	21.121993
257	C	10.952970	11.829885	17.542007
258	C	10.952970	11.829885	18.973993
259	C	9.902910	12.489690	19.690007
260	C	9.902910	12.489690	21.121993
261	C	8.732355	12.899280	17.542007
262	C	8.732355	12.899280	18.973993
263	C	7.500000	13.038135	19.690007
264	C	7.500000	13.038135	21.121993
265	C	6.267645	12.899280	17.542007
266	C	6.267645	12.899280	18.973993
267	C	5.097090	12.489690	19.690007

268	C	5.097090	12.489690	21.121993
269	C	4.047030	11.829885	17.542007
270	C	4.047030	11.829885	18.973993
271	C	3.170115	10.952970	19.690007
272	C	3.170115	10.952970	21.121993
273	C	2.510310	9.902910	17.542007
274	C	2.510310	9.902910	18.973993
275	C	2.100720	8.732355	19.690007
276	C	2.100720	8.732355	21.121993
277	C	1.961865	7.500000	17.542007
278	C	1.961865	7.500000	18.973993
279	C	2.100720	6.267645	19.690007
280	C	2.100720	6.267645	21.121993
281	C	2.510310	5.097090	17.542007
282	C	2.510310	5.097090	18.973993
283	C	3.170115	4.047030	19.690007
284	C	3.170115	4.047030	21.121993
285	C	4.047030	3.170115	17.542007
286	C	4.047030	3.170115	18.973993
287	C	5.097090	2.510310	19.690007
288	C	5.097090	2.510310	21.121993
289	C	6.267645	2.100720	17.542007
290	C	6.267645	2.100720	18.973993
291	C	7.500000	1.961865	19.690007
292	C	7.500000	1.961865	21.121993
293	C	8.732355	2.100720	17.542007
294	C	8.732355	2.100720	18.973993
295	C	9.902910	2.510310	19.690007
296	C	9.902910	2.510310	21.121993
297	C	10.952970	3.170115	17.542007
298	C	10.952970	3.170115	18.973993
299	C	11.829885	4.047030	19.690007
300	C	11.829885	4.047030	21.121993
301	C	12.489690	5.097090	17.542007
302	C	12.489690	5.097090	18.973993
303	C	12.899280	6.267645	19.690007
304	C	12.899280	6.267645	21.121993

Table S4. Calculated atomic positions for TP single-chain $TiTe_3$ encapsulated in a CNT.

The lengths of the lattice vectors are 15 Å, 15 Å, and 21.84 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	Ti	7.500000	7.500045	0.909287
2	Ti	7.500000	7.500435	4.548966
3	Ti	7.500000	7.503330	8.192381
4	Ti	7.500000	7.503915	11.829112
5	Ti	7.500000	7.501740	15.468857
6	Ti	7.500000	7.500300	19.112228
7	Te	7.500000	9.621240	2.733473
8	Te	7.500000	9.620790	6.367627
9	Te	7.500000	9.626340	10.008289
10	Te	7.500000	9.623400	13.654040
11	Te	7.500000	9.620175	17.288850
12	Te	7.500000	9.622725	20.928464
13	Te	9.345435	6.454620	2.733647
14	Te	9.341160	6.451905	6.368566
15	Te	9.343830	6.451200	10.008377
16	Te	9.341970	6.450540	13.653254
17	Te	9.342930	6.454395	17.288064
18	Te	9.346860	6.453285	20.928289
19	Te	5.654565	6.454620	2.733647
20	Te	5.658840	6.451905	6.368566
21	Te	5.656170	6.451200	10.008377
22	Te	5.658030	6.450540	13.653254
23	Te	5.657070	6.454395	17.288064
24	Te	5.653140	6.453285	20.928289
25	C	13.130955	7.500000	0.364007
26	C	13.130955	7.500000	1.819993
27	C	12.989775	8.753010	2.548007
28	C	12.989775	8.753010	4.003993
29	C	12.573315	9.943185	0.364007
30	C	12.573315	9.943185	1.819993
31	C	11.902455	11.010840	2.548007
32	C	11.902455	11.010840	4.003993
33	C	11.010840	11.902455	0.364007

34	C	11.010840	11.902455	1.819993
35	C	9.943185	12.573315	2.548007
36	C	9.943185	12.573315	4.003993
37	C	8.753010	12.989775	0.364007
38	C	8.753010	12.989775	1.819993
39	C	7.500000	13.130955	2.548007
40	C	7.500000	13.130955	4.003993
41	C	6.246990	12.989775	0.364007
42	C	6.246990	12.989775	1.819993
43	C	5.056815	12.573315	2.548007
44	C	5.056815	12.573315	4.003993
45	C	3.989160	11.902455	0.364007
46	C	3.989160	11.902455	1.819993
47	C	3.097545	11.010840	2.548007
48	C	3.097545	11.010840	4.003993
49	C	2.426685	9.943185	0.364007
50	C	2.426685	9.943185	1.819993
51	C	2.010225	8.753010	2.548007
52	C	2.010225	8.753010	4.003993
53	C	1.869045	7.500000	0.364007
54	C	1.869045	7.500000	1.819993
55	C	2.010225	6.246990	2.548007
56	C	2.010225	6.246990	4.003993
57	C	2.426685	5.056815	0.364007
58	C	2.426685	5.056815	1.819993
59	C	3.097545	3.989160	2.548007
60	C	3.097545	3.989160	4.003993
61	C	3.989160	3.097545	0.364007
62	C	3.989160	3.097545	1.819993
63	C	5.056815	2.426685	2.548007
64	C	5.056815	2.426685	4.003993
65	C	6.246990	2.010225	0.364007
66	C	6.246990	2.010225	1.819993
67	C	7.500000	1.869045	2.548007
68	C	7.500000	1.869045	4.003993
69	C	8.753010	2.010225	0.364007
70	C	8.753010	2.010225	1.819993
71	C	9.943185	2.426685	2.548007
72	C	9.943185	2.426685	4.003993

73	C	11.010840	3.097545	0.364007
74	C	11.010840	3.097545	1.819993
75	C	11.902455	3.989160	2.548007
76	C	11.902455	3.989160	4.003993
77	C	12.573315	5.056815	0.364007
78	C	12.573315	5.056815	1.819993
79	C	12.989775	6.246990	2.548007
80	C	12.989775	6.246990	4.003993
81	C	13.130955	7.500000	4.732007
82	C	13.130955	7.500000	6.187993
83	C	12.989775	8.753010	6.916007
84	C	12.989775	8.753010	8.371993
85	C	12.573315	9.943185	4.732007
86	C	12.573315	9.943185	6.187993
87	C	11.902455	11.010840	6.916007
88	C	11.902455	11.010840	8.371993
89	C	11.010840	11.902455	4.732007
90	C	11.010840	11.902455	6.187993
91	C	9.943185	12.573315	6.916007
92	C	9.943185	12.573315	8.371993
93	C	8.753010	12.989775	4.732007
94	C	8.753010	12.989775	6.187993
95	C	7.500000	13.130955	6.916007
96	C	7.500000	13.130955	8.371993
97	C	6.246990	12.989775	4.732007
98	C	6.246990	12.989775	6.187993
99	C	5.056815	12.573315	6.916007
100	C	5.056815	12.573315	8.371993
101	C	3.989160	11.902455	4.732007
102	C	3.989160	11.902455	6.187993
103	C	3.097545	11.010840	6.916007
104	C	3.097545	11.010840	8.371993
105	C	2.426685	9.943185	4.732007
106	C	2.426685	9.943185	6.187993
107	C	2.010225	8.753010	6.916007
108	C	2.010225	8.753010	8.371993
109	C	1.869045	7.500000	4.732007
110	C	1.869045	7.500000	6.187993
111	C	2.010225	6.246990	6.916007

112	C	2.010225	6.246990	8.371993
113	C	2.426685	5.056815	4.732007
114	C	2.426685	5.056815	6.187993
115	C	3.097545	3.989160	6.916007
116	C	3.097545	3.989160	8.371993
117	C	3.989160	3.097545	4.732007
118	C	3.989160	3.097545	6.187993
119	C	5.056815	2.426685	6.916007
120	C	5.056815	2.426685	8.371993
121	C	6.246990	2.010225	4.732007
122	C	6.246990	2.010225	6.187993
123	C	7.500000	1.869045	6.916007
124	C	7.500000	1.869045	8.371993
125	C	8.753010	2.010225	4.732007
126	C	8.753010	2.010225	6.187993
127	C	9.943185	2.426685	6.916007
128	C	9.943185	2.426685	8.371993
129	C	11.010840	3.097545	4.732007
130	C	11.010840	3.097545	6.187993
131	C	11.902455	3.989160	6.916007
132	C	11.902455	3.989160	8.371993
133	C	12.573315	5.056815	4.732007
134	C	12.573315	5.056815	6.187993
135	C	12.989775	6.246990	6.916007
136	C	12.989775	6.246990	8.371993
137	C	13.130955	7.500000	9.100007
138	C	13.130955	7.500000	10.555993
139	C	12.989775	8.753010	11.284007
140	C	12.989775	8.753010	12.739993
141	C	12.573315	9.943185	9.100007
142	C	12.573315	9.943185	10.555993
143	C	11.902455	11.010840	11.284007
144	C	11.902455	11.010840	12.739993
145	C	11.010840	11.902455	9.100007
146	C	11.010840	11.902455	10.555993
147	C	9.943185	12.573315	11.284007
148	C	9.943185	12.573315	12.739993
149	C	8.753010	12.989775	9.100007
150	C	8.753010	12.989775	10.555993

151	C	7.500000	13.130955	11.284007
152	C	7.500000	13.130955	12.739993
153	C	6.246990	12.989775	9.100007
154	C	6.246990	12.989775	10.555993
155	C	5.056815	12.573315	11.284007
156	C	5.056815	12.573315	12.739993
157	C	3.989160	11.902455	9.100007
158	C	3.989160	11.902455	10.555993
159	C	3.097545	11.010840	11.284007
160	C	3.097545	11.010840	12.739993
161	C	2.426685	9.943185	9.100007
162	C	2.426685	9.943185	10.555993
163	C	2.010225	8.753010	11.284007
164	C	2.010225	8.753010	12.739993
165	C	1.869045	7.500000	9.100007
166	C	1.869045	7.500000	10.555993
167	C	2.010225	6.246990	11.284007
168	C	2.010225	6.246990	12.739993
169	C	2.426685	5.056815	9.100007
170	C	2.426685	5.056815	10.555993
171	C	3.097545	3.989160	11.284007
172	C	3.097545	3.989160	12.739993
173	C	3.989160	3.097545	9.100007
174	C	3.989160	3.097545	10.555993
175	C	5.056815	2.426685	11.284007
176	C	5.056815	2.426685	12.739993
177	C	6.246990	2.010225	9.100007
178	C	6.246990	2.010225	10.555993
179	C	7.500000	1.869045	11.284007
180	C	7.500000	1.869045	12.739993
181	C	8.753010	2.010225	9.100007
182	C	8.753010	2.010225	10.555993
183	C	9.943185	2.426685	11.284007
184	C	9.943185	2.426685	12.739993
185	C	11.010840	3.097545	9.100007
186	C	11.010840	3.097545	10.555993
187	C	11.902455	3.989160	11.284007
188	C	11.902455	3.989160	12.739993
189	C	12.573315	5.056815	9.100007

190	C	12.573315	5.056815	10.555993
191	C	12.989775	6.246990	11.284007
192	C	12.989775	6.246990	12.739993
193	C	13.130955	7.500000	13.468007
194	C	13.130955	7.500000	14.923993
195	C	12.989775	8.753010	15.652007
196	C	12.989775	8.753010	17.107993
197	C	12.573315	9.943185	13.468007
198	C	12.573315	9.943185	14.923993
199	C	11.902455	11.010840	15.652007
200	C	11.902455	11.010840	17.107993
201	C	11.010840	11.902455	13.468007
202	C	11.010840	11.902455	14.923993
203	C	9.943185	12.573315	15.652007
204	C	9.943185	12.573315	17.107993
205	C	8.753010	12.989775	13.468007
206	C	8.753010	12.989775	14.923993
207	C	7.500000	13.130955	15.652007
208	C	7.500000	13.130955	17.107993
209	C	6.246990	12.989775	13.468007
210	C	6.246990	12.989775	14.923993
211	C	5.056815	12.573315	15.652007
212	C	5.056815	12.573315	17.107993
213	C	3.989160	11.902455	13.468007
214	C	3.989160	11.902455	14.923993
215	C	3.097545	11.010840	15.652007
216	C	3.097545	11.010840	17.107993
217	C	2.426685	9.943185	13.468007
218	C	2.426685	9.943185	14.923993
219	C	2.010225	8.753010	15.652007
220	C	2.010225	8.753010	17.107993
221	C	1.869045	7.500000	13.468007
222	C	1.869045	7.500000	14.923993
223	C	2.010225	6.246990	15.652007
224	C	2.010225	6.246990	17.107993
225	C	2.426685	5.056815	13.468007
226	C	2.426685	5.056815	14.923993
227	C	3.097545	3.989160	15.652007
228	C	3.097545	3.989160	17.107993

229	C	3.989160	3.097545	13.468007
230	C	3.989160	3.097545	14.923993
231	C	5.056815	2.426685	15.652007
232	C	5.056815	2.426685	17.107993
233	C	6.246990	2.010225	13.468007
234	C	6.246990	2.010225	14.923993
235	C	7.500000	1.869045	15.652007
236	C	7.500000	1.869045	17.107993
237	C	8.753010	2.010225	13.468007
238	C	8.753010	2.010225	14.923993
239	C	9.943185	2.426685	15.652007
240	C	9.943185	2.426685	17.107993
241	C	11.010840	3.097545	13.468007
242	C	11.010840	3.097545	14.923993
243	C	11.902455	3.989160	15.652007
244	C	11.902455	3.989160	17.107993
245	C	12.573315	5.056815	13.468007
246	C	12.573315	5.056815	14.923993
247	C	12.989775	6.246990	15.652007
248	C	12.989775	6.246990	17.107993
249	C	13.130955	7.500000	17.836007
250	C	13.130955	7.500000	19.291993
251	C	12.989775	8.753010	20.020007
252	C	12.989775	8.753010	21.475993
253	C	12.573315	9.943185	17.836007
254	C	12.573315	9.943185	19.291993
255	C	11.902455	11.010840	20.020007
256	C	11.902455	11.010840	21.475993
257	C	11.010840	11.902455	17.836007
258	C	11.010840	11.902455	19.291993
259	C	9.943185	12.573315	20.020007
260	C	9.943185	12.573315	21.475993
261	C	8.753010	12.989775	17.836007
262	C	8.753010	12.989775	19.291993
263	C	7.500000	13.130955	20.020007
264	C	7.500000	13.130955	21.475993
265	C	6.246990	12.989775	17.836007
266	C	6.246990	12.989775	19.291993
267	C	5.056815	12.573315	20.020007

268	C	5.056815	12.573315	21.475993
269	C	3.989160	11.902455	17.836007
270	C	3.989160	11.902455	19.291993
271	C	3.097545	11.010840	20.020007
272	C	3.097545	11.010840	21.475993
273	C	2.426685	9.943185	17.836007
274	C	2.426685	9.943185	19.291993
275	C	2.010225	8.753010	20.020007
276	C	2.010225	8.753010	21.475993
277	C	1.869045	7.500000	17.836007
278	C	1.869045	7.500000	19.291993
279	C	2.010225	6.246990	20.020007
280	C	2.010225	6.246990	21.475993
281	C	2.426685	5.056815	17.836007
282	C	2.426685	5.056815	19.291993
283	C	3.097545	3.989160	20.020007
284	C	3.097545	3.989160	21.475993
285	C	3.989160	3.097545	17.836007
286	C	3.989160	3.097545	19.291993
287	C	5.056815	2.426685	20.020007
288	C	5.056815	2.426685	21.475993
289	C	6.246990	2.010225	17.836007
290	C	6.246990	2.010225	19.291993
291	C	7.500000	1.869045	20.020007
292	C	7.500000	1.869045	21.475993
293	C	8.753010	2.010225	17.836007
294	C	8.753010	2.010225	19.291993
295	C	9.943185	2.426685	20.020007
296	C	9.943185	2.426685	21.475993
297	C	11.010840	3.097545	17.836007
298	C	11.010840	3.097545	19.291993
299	C	11.902455	3.989160	20.020007
300	C	11.902455	3.989160	21.475993
301	C	12.573315	5.056815	17.836007
302	C	12.573315	5.056815	19.291993
303	C	12.989775	6.246990	20.020007
304	C	12.989775	6.246990	21.475993

Table S5. Calculated atomic positions for TP single-chain VTe_3 encapsulated in a CNT. The lengths of the lattice vectors are 15 Å, 15 Å, and 13.62 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	V	7.500000	7.496850	0.389178
2	V	7.500000	7.496145	3.795513
3	V	7.500000	7.496820	7.199001
4	V	7.500000	7.496115	10.605499
5	Te	7.500000	9.083760	2.091841
6	Te	8.865195	6.693825	2.091692
7	Te	6.134805	6.693825	2.091705
8	Te	7.500000	9.084525	5.498530
9	Te	8.866185	6.693675	5.498394
10	Te	6.133815	6.693675	5.498394
11	Te	7.500000	9.083790	8.901678
12	Te	8.865240	6.693855	8.901719
13	Te	6.134760	6.693855	8.901719
14	Te	7.500000	9.084570	12.308435
15	Te	8.866365	6.693930	12.308544
16	Te	6.133635	6.693930	12.308530
17	C	11.889510	7.500000	0.378336
18	C	11.889510	7.500000	1.891668
19	C	11.779455	8.476755	2.648327
20	C	11.779455	8.476755	4.161673
21	C	11.454810	9.404535	0.378336
22	C	11.454810	9.404535	1.891668
23	C	10.931865	10.236810	2.648327
24	C	10.931865	10.236810	4.161673
25	C	10.236810	10.931865	0.378336
26	C	10.236810	10.931865	1.891668
27	C	9.404535	11.454810	2.648327
28	C	9.404535	11.454810	4.161673
29	C	8.476755	11.779455	0.378336
30	C	8.476755	11.779455	1.891668
31	C	7.500000	11.889510	2.648327
32	C	7.500000	11.889510	4.161673
33	C	6.523245	11.779455	0.378336
34	C	6.523245	11.779455	1.891668

35	C	5.595465	11.454810	2.648327
36	C	5.595465	11.454810	4.161673
37	C	4.763190	10.931865	0.378336
38	C	4.763190	10.931865	1.891668
39	C	4.068135	10.236810	2.648327
40	C	4.068135	10.236810	4.161673
41	C	3.545190	9.404535	0.378336
42	C	3.545190	9.404535	1.891668
43	C	3.220545	8.476755	2.648327
44	C	3.220545	8.476755	4.161673
45	C	3.110490	7.500000	0.378336
46	C	3.110490	7.500000	1.891668
47	C	3.220545	6.523245	2.648327
48	C	3.220545	6.523245	4.161673
49	C	3.545190	5.595465	0.378336
50	C	3.545190	5.595465	1.891668
51	C	4.068135	4.763190	2.648327
52	C	4.068135	4.763190	4.161673
53	C	4.763190	4.068135	0.378336
54	C	4.763190	4.068135	1.891668
55	C	5.595465	3.545190	2.648327
56	C	5.595465	3.545190	4.161673
57	C	6.523245	3.220545	0.378336
58	C	6.523245	3.220545	1.891668
59	C	7.500000	3.110490	2.648327
60	C	7.500000	3.110490	4.161673
61	C	8.476755	3.220545	0.378336
62	C	8.476755	3.220545	1.891668
63	C	9.404535	3.545190	2.648327
64	C	9.404535	3.545190	4.161673
65	C	10.236810	4.068135	0.378336
66	C	10.236810	4.068135	1.891668
67	C	10.931865	4.763190	2.648327
68	C	10.931865	4.763190	4.161673
69	C	11.454810	5.595465	0.378336
70	C	11.454810	5.595465	1.891668
71	C	11.779455	6.523245	2.648327
72	C	11.779455	6.523245	4.161673
73	C	11.889510	7.500000	4.918332

74	C	11.889510	7.500000	6.431664
75	C	11.779455	8.476755	7.188336
76	C	11.779455	8.476755	8.701668
77	C	11.454810	9.404535	4.918332
78	C	11.454810	9.404535	6.431664
79	C	10.931865	10.236810	7.188336
80	C	10.931865	10.236810	8.701668
81	C	10.236810	10.931865	4.918332
82	C	10.236810	10.931865	6.431664
83	C	9.404535	11.454810	7.188336
84	C	9.404535	11.454810	8.701668
85	C	8.476755	11.779455	4.918332
86	C	8.476755	11.779455	6.431664
87	C	7.500000	11.889510	7.188336
88	C	7.500000	11.889510	8.701668
89	C	6.523245	11.779455	4.918332
90	C	6.523245	11.779455	6.431664
91	C	5.595465	11.454810	7.188336
92	C	5.595465	11.454810	8.701668
93	C	4.763190	10.931865	4.918332
94	C	4.763190	10.931865	6.431664
95	C	4.068135	10.236810	7.188336
96	C	4.068135	10.236810	8.701668
97	C	3.545190	9.404535	4.918332
98	C	3.545190	9.404535	6.431664
99	C	3.220545	8.476755	7.188336
100	C	3.220545	8.476755	8.701668
101	C	3.110490	7.500000	4.918332
102	C	3.110490	7.500000	6.431664
103	C	3.220545	6.523245	7.188336
104	C	3.220545	6.523245	8.701668
105	C	3.545190	5.595465	4.918332
106	C	3.545190	5.595465	6.431664
107	C	4.068135	4.763190	7.188336
108	C	4.068135	4.763190	8.701668
109	C	4.763190	4.068135	4.918332
110	C	4.763190	4.068135	6.431664
111	C	5.595465	3.545190	7.188336
112	C	5.595465	3.545190	8.701668

113	C	6.523245	3.220545	4.918332
114	C	6.523245	3.220545	6.431664
115	C	7.500000	3.110490	7.188336
116	C	7.500000	3.110490	8.701668
117	C	8.476755	3.220545	4.918332
118	C	8.476755	3.220545	6.431664
119	C	9.404535	3.545190	7.188336
120	C	9.404535	3.545190	8.701668
121	C	10.236810	4.068135	4.918332
122	C	10.236810	4.068135	6.431664
123	C	10.931865	4.763190	7.188336
124	C	10.931865	4.763190	8.701668
125	C	11.454810	5.595465	4.918332
126	C	11.454810	5.595465	6.431664
127	C	11.779455	6.523245	7.188336
128	C	11.779455	6.523245	8.701668
129	C	11.889510	7.500000	9.458327
130	C	11.889510	7.500000	10.971673
131	C	11.779455	8.476755	11.728332
132	C	11.779455	8.476755	13.241664
133	C	11.454810	9.404535	9.458327
134	C	11.454810	9.404535	10.971673
135	C	10.931865	10.236810	11.728332
136	C	10.931865	10.236810	13.241664
137	C	10.236810	10.931865	9.458327
138	C	10.236810	10.931865	10.971673
139	C	9.404535	11.454810	11.728332
140	C	9.404535	11.454810	13.241664
141	C	8.476755	11.779455	9.458327
142	C	8.476755	11.779455	10.971673
143	C	7.500000	11.889510	11.728332
144	C	7.500000	11.889510	13.241664
145	C	6.523245	11.779455	9.458327
146	C	6.523245	11.779455	10.971673
147	C	5.595465	11.454810	11.728332
148	C	5.595465	11.454810	13.241664
149	C	4.763190	10.931865	9.458327
150	C	4.763190	10.931865	10.971673
151	C	4.068135	10.236810	11.728332

152	C	4.068135	10.236810	13.241664
153	C	3.545190	9.404535	9.458327
154	C	3.545190	9.404535	10.971673
155	C	3.220545	8.476755	11.728332
156	C	3.220545	8.476755	13.241664
157	C	3.110490	7.500000	9.458327
158	C	3.110490	7.500000	10.971673
159	C	3.220545	6.523245	11.728332
160	C	3.220545	6.523245	13.241664
161	C	3.545190	5.595465	9.458327
162	C	3.545190	5.595465	10.971673
163	C	4.068135	4.763190	11.728332
164	C	4.068135	4.763190	13.241664
165	C	4.763190	4.068135	9.458327
166	C	4.763190	4.068135	10.971673
167	C	5.595465	3.545190	11.728332
168	C	5.595465	3.545190	13.241664
169	C	6.523245	3.220545	9.458327
170	C	6.523245	3.220545	10.971673
171	C	7.500000	3.110490	11.728332
172	C	7.500000	3.110490	13.241664
173	C	8.476755	3.220545	9.458327
174	C	8.476755	3.220545	10.971673
175	C	9.404535	3.545190	11.728332
176	C	9.404535	3.545190	13.241664
177	C	10.236810	4.068135	9.458327
178	C	10.236810	4.068135	10.971673
179	C	10.931865	4.763190	11.728332
180	C	10.931865	4.763190	13.241664
181	C	11.454810	5.595465	9.458327
182	C	11.454810	5.595465	10.971673
183	C	11.779455	6.523245	11.728332
184	C	11.779455	6.523245	13.241664

Table S6. Calculated atomic positions for TP single-chain $NbTe_3$ encapsulated in a CNT.

The lengths of the lattice vectors are 15 Å, 15 Å, and 21.48 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	Nb	7.500000	7.496505	0.463238
2	Nb	7.500000	7.495860	4.045951
3	Nb	7.500000	7.494390	7.625400
4	Nb	7.500000	7.495575	11.203087
5	Nb	7.500000	7.496250	14.785822
6	Nb	7.500000	7.495935	18.365336
7	Te	7.500000	9.685755	2.257698
8	Te	7.500000	9.686865	5.829393
9	Te	7.500000	9.687585	9.418830
10	Te	7.500000	9.685560	12.996775
11	Te	7.500000	9.687345	16.568770
12	Te	7.500000	9.688320	20.159152
13	Te	9.394290	6.399120	2.256882
14	Te	9.395865	6.396195	5.828426
15	Te	9.397455	6.396435	9.419603
16	Te	9.394245	6.398745	12.997419
17	Te	9.396120	6.397395	16.568877
18	Te	9.397425	6.397380	20.159410
19	Te	5.605710	6.399120	2.256882
20	Te	5.604135	6.396195	5.828426
21	Te	5.602545	6.396435	9.419603
22	Te	5.605755	6.398745	12.997419
23	Te	5.603880	6.397395	16.568877
24	Te	5.602575	6.397380	20.159431
25	C	13.038135	7.500000	0.358007
26	C	13.038135	7.500000	1.789993
27	C	12.899280	8.732355	2.506007
28	C	12.899280	8.732355	3.937993
29	C	12.489690	9.902910	0.358007
30	C	12.489690	9.902910	1.789993
31	C	11.829885	10.952970	2.506007
32	C	11.829885	10.952970	3.937993
33	C	10.952970	11.829885	0.358007

34	C	10.952970	11.829885	1.789993
35	C	9.902910	12.489690	2.506007
36	C	9.902910	12.489690	3.937993
37	C	8.732355	12.899280	0.358007
38	C	8.732355	12.899280	1.789993
39	C	7.500000	13.038135	2.506007
40	C	7.500000	13.038135	3.937993
41	C	6.267645	12.899280	0.358007
42	C	6.267645	12.899280	1.789993
43	C	5.097090	12.489690	2.506007
44	C	5.097090	12.489690	3.937993
45	C	4.047030	11.829885	0.358007
46	C	4.047030	11.829885	1.789993
47	C	3.170115	10.952970	2.506007
48	C	3.170115	10.952970	3.937993
49	C	2.510310	9.902910	0.358007
50	C	2.510310	9.902910	1.789993
51	C	2.100720	8.732355	2.506007
52	C	2.100720	8.732355	3.937993
53	C	1.961865	7.500000	0.358007
54	C	1.961865	7.500000	1.789993
55	C	2.100720	6.267645	2.506007
56	C	2.100720	6.267645	3.937993
57	C	2.510310	5.097090	0.358007
58	C	2.510310	5.097090	1.789993
59	C	3.170115	4.047030	2.506007
60	C	3.170115	4.047030	3.937993
61	C	4.047030	3.170115	0.358007
62	C	4.047030	3.170115	1.789993
63	C	5.097090	2.510310	2.506007
64	C	5.097090	2.510310	3.937993
65	C	6.267645	2.100720	0.358007
66	C	6.267645	2.100720	1.789993
67	C	7.500000	1.961865	2.506007
68	C	7.500000	1.961865	3.937993
69	C	8.732355	2.100720	0.358007
70	C	8.732355	2.100720	1.789993
71	C	9.902910	2.510310	2.506007
72	C	9.902910	2.510310	3.937993

73	C	10.952970	3.170115	0.358007
74	C	10.952970	3.170115	1.789993
75	C	11.829885	4.047030	2.506007
76	C	11.829885	4.047030	3.937993
77	C	12.489690	5.097090	0.358007
78	C	12.489690	5.097090	1.789993
79	C	12.899280	6.267645	2.506007
80	C	12.899280	6.267645	3.937993
81	C	13.038135	7.500000	4.654007
82	C	13.038135	7.500000	6.085993
83	C	12.899280	8.732355	6.802007
84	C	12.899280	8.732355	8.233993
85	C	12.489690	9.902910	4.654007
86	C	12.489690	9.902910	6.085993
87	C	11.829885	10.952970	6.802007
88	C	11.829885	10.952970	8.233993
89	C	10.952970	11.829885	4.654007
90	C	10.952970	11.829885	6.085993
91	C	9.902910	12.489690	6.802007
92	C	9.902910	12.489690	8.233993
93	C	8.732355	12.899280	4.654007
94	C	8.732355	12.899280	6.085993
95	C	7.500000	13.038135	6.802007
96	C	7.500000	13.038135	8.233993
97	C	6.267645	12.899280	4.654007
98	C	6.267645	12.899280	6.085993
99	C	5.097090	12.489690	6.802007
100	C	5.097090	12.489690	8.233993
101	C	4.047030	11.829885	4.654007
102	C	4.047030	11.829885	6.085993
103	C	3.170115	10.952970	6.802007
104	C	3.170115	10.952970	8.233993
105	C	2.510310	9.902910	4.654007
106	C	2.510310	9.902910	6.085993
107	C	2.100720	8.732355	6.802007
108	C	2.100720	8.732355	8.233993
109	C	1.961865	7.500000	4.654007
110	C	1.961865	7.500000	6.085993
111	C	2.100720	6.267645	6.802007

112	C	2.100720	6.267645	8.233993
113	C	2.510310	5.097090	4.654007
114	C	2.510310	5.097090	6.085993
115	C	3.170115	4.047030	6.802007
116	C	3.170115	4.047030	8.233993
117	C	4.047030	3.170115	4.654007
118	C	4.047030	3.170115	6.085993
119	C	5.097090	2.510310	6.802007
120	C	5.097090	2.510310	8.233993
121	C	6.267645	2.100720	4.654007
122	C	6.267645	2.100720	6.085993
123	C	7.500000	1.961865	6.802007
124	C	7.500000	1.961865	8.233993
125	C	8.732355	2.100720	4.654007
126	C	8.732355	2.100720	6.085993
127	C	9.902910	2.510310	6.802007
128	C	9.902910	2.510310	8.233993
129	C	10.952970	3.170115	4.654007
130	C	10.952970	3.170115	6.085993
131	C	11.829885	4.047030	6.802007
132	C	11.829885	4.047030	8.233993
133	C	12.489690	5.097090	4.654007
134	C	12.489690	5.097090	6.085993
135	C	12.899280	6.267645	6.802007
136	C	12.899280	6.267645	8.233993
137	C	13.038135	7.500000	8.950007
138	C	13.038135	7.500000	10.381993
139	C	12.899280	8.732355	11.098007
140	C	12.899280	8.732355	12.529993
141	C	12.489690	9.902910	8.950007
142	C	12.489690	9.902910	10.381993
143	C	11.829885	10.952970	11.098007
144	C	11.829885	10.952970	12.529993
145	C	10.952970	11.829885	8.950007
146	C	10.952970	11.829885	10.381993
147	C	9.902910	12.489690	11.098007
148	C	9.902910	12.489690	12.529993
149	C	8.732355	12.899280	8.950007
150	C	8.732355	12.899280	10.381993

151	C	7.500000	13.038135	11.098007
152	C	7.500000	13.038135	12.529993
153	C	6.267645	12.899280	8.950007
154	C	6.267645	12.899280	10.381993
155	C	5.097090	12.489690	11.098007
156	C	5.097090	12.489690	12.529993
157	C	4.047030	11.829885	8.950007
158	C	4.047030	11.829885	10.381993
159	C	3.170115	10.952970	11.098007
160	C	3.170115	10.952970	12.529993
161	C	2.510310	9.902910	8.950007
162	C	2.510310	9.902910	10.381993
163	C	2.100720	8.732355	11.098007
164	C	2.100720	8.732355	12.529993
165	C	1.961865	7.500000	8.950007
166	C	1.961865	7.500000	10.381993
167	C	2.100720	6.267645	11.098007
168	C	2.100720	6.267645	12.529993
169	C	2.510310	5.097090	8.950007
170	C	2.510310	5.097090	10.381993
171	C	3.170115	4.047030	11.098007
172	C	3.170115	4.047030	12.529993
173	C	4.047030	3.170115	8.950007
174	C	4.047030	3.170115	10.381993
175	C	5.097090	2.510310	11.098007
176	C	5.097090	2.510310	12.529993
177	C	6.267645	2.100720	8.950007
178	C	6.267645	2.100720	10.381993
179	C	7.500000	1.961865	11.098007
180	C	7.500000	1.961865	12.529993
181	C	8.732355	2.100720	8.950007
182	C	8.732355	2.100720	10.381993
183	C	9.902910	2.510310	11.098007
184	C	9.902910	2.510310	12.529993
185	C	10.952970	3.170115	8.950007
186	C	10.952970	3.170115	10.381993
187	C	11.829885	4.047030	11.098007
188	C	11.829885	4.047030	12.529993
189	C	12.489690	5.097090	8.950007

190	C	12.489690	5.097090	10.381993
191	C	12.899280	6.267645	11.098007
192	C	12.899280	6.267645	12.529993
193	C	13.038135	7.500000	13.246007
194	C	13.038135	7.500000	14.677993
195	C	12.899280	8.732355	15.394007
196	C	12.899280	8.732355	16.825993
197	C	12.489690	9.902910	13.246007
198	C	12.489690	9.902910	14.677993
199	C	11.829885	10.952970	15.394007
200	C	11.829885	10.952970	16.825993
201	C	10.952970	11.829885	13.246007
202	C	10.952970	11.829885	14.677993
203	C	9.902910	12.489690	15.394007
204	C	9.902910	12.489690	16.825993
205	C	8.732355	12.899280	13.246007
206	C	8.732355	12.899280	14.677993
207	C	7.500000	13.038135	15.394007
208	C	7.500000	13.038135	16.825993
209	C	6.267645	12.899280	13.246007
210	C	6.267645	12.899280	14.677993
211	C	5.097090	12.489690	15.394007
212	C	5.097090	12.489690	16.825993
213	C	4.047030	11.829885	13.246007
214	C	4.047030	11.829885	14.677993
215	C	3.170115	10.952970	15.394007
216	C	3.170115	10.952970	16.825993
217	C	2.510310	9.902910	13.246007
218	C	2.510310	9.902910	14.677993
219	C	2.100720	8.732355	15.394007
220	C	2.100720	8.732355	16.825993
221	C	1.961865	7.500000	13.246007
222	C	1.961865	7.500000	14.677993
223	C	2.100720	6.267645	15.394007
224	C	2.100720	6.267645	16.825993
225	C	2.510310	5.097090	13.246007
226	C	2.510310	5.097090	14.677993
227	C	3.170115	4.047030	15.394007
228	C	3.170115	4.047030	16.825993

229	C	4.047030	3.170115	13.246007
230	C	4.047030	3.170115	14.677993
231	C	5.097090	2.510310	15.394007
232	C	5.097090	2.510310	16.825993
233	C	6.267645	2.100720	13.246007
234	C	6.267645	2.100720	14.677993
235	C	7.500000	1.961865	15.394007
236	C	7.500000	1.961865	16.825993
237	C	8.732355	2.100720	13.246007
238	C	8.732355	2.100720	14.677993
239	C	9.902910	2.510310	15.394007
240	C	9.902910	2.510310	16.825993
241	C	10.952970	3.170115	13.246007
242	C	10.952970	3.170115	14.677993
243	C	11.829885	4.047030	15.394007
244	C	11.829885	4.047030	16.825993
245	C	12.489690	5.097090	13.246007
246	C	12.489690	5.097090	14.677993
247	C	12.899280	6.267645	15.394007
248	C	12.899280	6.267645	16.825993
249	C	13.038135	7.500000	17.542007
250	C	13.038135	7.500000	18.973993
251	C	12.899280	8.732355	19.690007
252	C	12.899280	8.732355	21.121993
253	C	12.489690	9.902910	17.542007
254	C	12.489690	9.902910	18.973993
255	C	11.829885	10.952970	19.690007
256	C	11.829885	10.952970	21.121993
257	C	10.952970	11.829885	17.542007
258	C	10.952970	11.829885	18.973993
259	C	9.902910	12.489690	19.690007
260	C	9.902910	12.489690	21.121993
261	C	8.732355	12.899280	17.542007
262	C	8.732355	12.899280	18.973993
263	C	7.500000	13.038135	19.690007
264	C	7.500000	13.038135	21.121993
265	C	6.267645	12.899280	17.542007
266	C	6.267645	12.899280	18.973993
267	C	5.097090	12.489690	19.690007

268	C	5.097090	12.489690	21.121993
269	C	4.047030	11.829885	17.542007
270	C	4.047030	11.829885	18.973993
271	C	3.170115	10.952970	19.690007
272	C	3.170115	10.952970	21.121993
273	C	2.510310	9.902910	17.542007
274	C	2.510310	9.902910	18.973993
275	C	2.100720	8.732355	19.690007
276	C	2.100720	8.732355	21.121993
277	C	1.961865	7.500000	17.542007
278	C	1.961865	7.500000	18.973993
279	C	2.100720	6.267645	19.690007
280	C	2.100720	6.267645	21.121993
281	C	2.510310	5.097090	17.542007
282	C	2.510310	5.097090	18.973993
283	C	3.170115	4.047030	19.690007
284	C	3.170115	4.047030	21.121993
285	C	4.047030	3.170115	17.542007
286	C	4.047030	3.170115	18.973993
287	C	5.097090	2.510310	19.690007
288	C	5.097090	2.510310	21.121993
289	C	6.267645	2.100720	17.542007
290	C	6.267645	2.100720	18.973993
291	C	7.500000	1.961865	19.690007
292	C	7.500000	1.961865	21.121993
293	C	8.732355	2.100720	17.542007
294	C	8.732355	2.100720	18.973993
295	C	9.902910	2.510310	19.690007
296	C	9.902910	2.510310	21.121993
297	C	10.952970	3.170115	17.542007
298	C	10.952970	3.170115	18.973993
299	C	11.829885	4.047030	19.690007
300	C	11.829885	4.047030	21.121993
301	C	12.489690	5.097090	17.542007
302	C	12.489690	5.097090	18.973993
303	C	12.899280	6.267645	19.690007
304	C	12.899280	6.267645	21.121993

Table S7. Calculated atomic positions for TAP single-chain $TiTe_3$ isolated in vacuum. The lengths of the lattice vectors are 30 Å, 30 Å, and 7.28 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	Ti	14.781360	14.672010	0.454534
2	Ti	14.781420	14.671950	4.095386
3	Te	16.983990	14.533500	2.274898
4	Te	15.465060	16.869210	2.275051
5	Te	12.995370	13.856250	2.275044
6	Te	16.411260	16.296930	5.914978
7	Te	13.638870	16.561680	5.914920
8	Te	14.891670	12.711150	5.914971

Table S8. Calculated atomic positions for TAP single-chain VTe_3 isolated in vacuum. The lengths of the lattice vectors are 30 Å, 30 Å, and 6.81 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	V	14.825520	14.672550	0.438578
2	Te	16.987770	14.431620	2.104515
3	Te	15.519870	16.821780	2.104760
4	Te	12.912840	13.963500	2.104699
5	V	14.825520	14.672610	3.770731
6	Te	16.358190	16.297500	5.509624
7	Te	13.581780	16.446480	5.509651
8	Te	15.048300	12.689100	5.509760

Table S9. Calculated atomic positions for TAP single-chain $NbTe_3$ isolated in vacuum. The lengths of the lattice vectors are 30 Å, 30 Å, and 7.16 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	Nb	14.822190	14.586720	0.600874
2	Te	17.187420	14.580660	2.243679
3	Te	15.568290	16.903080	2.243307
4	Te	12.700470	13.906140	2.243808
5	Nb	14.822280	14.586300	3.885682
6	Te	16.409280	16.254030	5.823586
7	Te	13.633290	16.483110	5.821925
8	Te	15.003600	12.549990	5.824008

Table S10. Calculated atomic positions for TP single-chain $TiTe_3$ isolated in vacuum. The lengths of the lattice vectors are 30 Å, 30 Å, and 3.64 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	Ti	15.000000	14.815950	0.910000
2	Te	15.000000	16.935810	2.730000
3	Te	13.082250	13.900470	2.730000
4	Te	16.917750	13.900470	2.730000

Table S11. Calculated atomic positions for TP single-chain VTe_3 isolated in vacuum. The lengths of the lattice vectors are 30 Å, 30 Å, and 3.405 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	V	15.000000	14.978100	0.851250
2	Te	15.000000	12.870690	2.553750
3	Te	16.822290	16.036020	2.553750
4	Te	13.177710	16.036020	2.553750

Table S12. Calculated atomic positions for TP single-chain $NbTe_3$ isolated in vacuum. The lengths of the lattice vectors are 30 Å, 30 Å, and 3.58 Å in x, y, and z directions, respectively.

	Species	x (Å)	y (Å)	z (Å)
1	Nb	15.000000	14.983560	0.895000
2	Te	15.000000	12.766590	2.685000
3	Te	16.920720	16.091340	2.685000
4	Te	13.079280	16.091340	2.685000