Supporting information for the manuscript entitled

"Field emission signature of pentagons at carbon nanotube caps"

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Some of the commands that we set for our electronic structure calculation with Siesta + atomic coordinates of the caps

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NumberOfAtoms       122
NumberOfSpecies     1
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 1  6  C      # Species index, atomic number, species label
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XC.authors = PBE
#############################
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SolutionMethod = diagon
MeshCutoff = 150 Ry
#############################
PAO.EnergyShift= 0.0045 Ry
#############################
DM.NumberKick = 20  # skip mixing every numberkick steps
DM.NumberPulay = 10  # last number of steps used in pulay mixing
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DM.Tolerance=0.00001
#############################
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  -3.76963973   -1.24774013    6.57934512   1  C        27
  -2.32192808   -3.20174388    6.44018285   1  C        28
    .02840202   -3.96930434    6.57741238   1  C       29
   2.33460030   -3.20320522    6.45019211   1  C        30
   2.39601701    3.36586518   12.25380127   1  C        31
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1.24194531	3.83543435	12.95422560	1	C	32
.05092649	4.11347620	12.18765579	1	C	33
-1.09543050	3.72651477	12.95792221	1	C	34
-.59588586	3.31353429	14.25703448	1	C	35
.85592679	3.31936303	14.24751639	1	C	36
1.60483953	2.27269206	14.89392498	1	C	37
2.82794996	1.89383254	14.24411627	1	C	38
3.19270802	2.41570781	12.95137704	1	C	39
3.84793366	1.37736095	12.18257188	1	C	40
3.85701785	.18652053	12.95594455	1	C	41
3.31181739	.52261918	14.25666167	1	C	42
-2.20509358	3.11284874	12.31306101	1	C	43
-2.93239775	2.09625557	13.06996126	1	C	44
-2.50572210	1.77908043	14.39963218	1	C	45
-1.29640350	2.33812634	14.96243242	1	C	46
-.57793750	1.29225939	15.68972422	1	C	47
.85380330	1.22866292	15.62348040	1	C	48
1.39300130	-.10430807	15.68514954	1	C	49
2.61523210	-.45090329	14.95727472	1	C	50
2.51086630	-1.77913065	14.39959802	1	C	51
2.93417335	-2.09348804	13.06897797	1	C	52
3.64077604	-1.07012132	12.31135023	1	C	53
1.30003726	-2.33774682	14.95952135	1	C	54
.57976853	-1.29138307	15.68920765	1	C	55
-.85132075	-1.22762443	15.62207691	1	C	56
-1.39005244	.10449619	15.68476709	1	C	57
-2.61333499	.45220334	14.95622868	1	C	58
-3.64052514	1.07474067	12.31785877	1	C	59
-3.85360940	-.18475498	12.95543114	1	C	60
-3.31223003	-.52093208	14.25622914	1	C	61
-2.82482329	-1.89177949	14.24229566	1	C	62
-1.60310870	-2.27265297	14.89183394	1	C	63
-.85415044	-3.31936227	14.24625778	1	C	64
.59838930	-3.31418628	14.25652180	1	C	65
1.09553906	-3.72385945	12.95662859	1	C	66
2.20675980	-3.11089187	12.31950014	1	C	67
-.05215214	-4.11095981	12.17778062	1	C	68
-1.24156625	-3.83738743	12.95438709	1	C	69
-2.39947829	-3.37088684	12.26609223	1	C	70
-3.19342583	-2.41477504	12.95130468	1	C	71
-3.84626354	-1.37699142	12.17494697	1	C	72
3.78395137	1.28024725	7.92548104	1	C	73
2.33665949	3.26119173	7.96636844	1	C	74
-.01398291	4.02225485	7.92305096	1	C	75
-2.33273404	3.19792869	7.99809359	1	C	76
-3.96631952	-.06341993	10.10128565	1	C	77

-3.96694927	-.02193042	8.66754249	1	C	78
-3.84910474	-1.35437379	10.76652389	1	C	79
-3.25236255	-2.47297685	10.08256405	1	C	80
-3.20439920	-2.41018205	8.65827277	1	C	81
-2.40893592	-3.38427091	10.81414294	1	C	82
-1.27963346	-3.90014067	10.08175081	1	C	83
-1.24677172	-3.83904303	8.65416096	1	C	84
-.02451581	-4.10436082	10.77085640	1	C	85
1.23225747	-3.79732248	10.10303131	1	C	86
1.24978535	-3.77875598	8.66907534	1	C	87
2.28411917	-3.17827069	10.86971877	1	C	88
3.15090770	-2.27131590	10.14985048	1	C	89
3.18163279	-2.29567272	8.70828530	1	C	90
3.71245803	-1.12424411	10.86453649	1	C	91
3.96686851	.07624012	10.10286517	1	C	92
-3.71482027	1.12985793	10.86872476	1	C	93
-3.19338287	2.28343846	8.70757082	1	C	94
-3.17048697	2.27077470	10.15111261	1	C	95
-2.28652980	3.18503072	10.86510128	1	C	96
-1.23380779	3.82437512	8.66838519	1	C	97
-1.23185429	3.83091676	10.10541838	1	C	98
.01717344	4.11290238	10.78378036	1	C	99
1.22638167	3.84777469	8.65461582	1	C	100
1.25598785	3.90010440	10.08447954	1	C	101
2.40444659	3.38238027	10.80373076	1	C	102
3.24551868	2.40633561	8.65837894	1	C	103
3.26696352	2.46698152	10.08375176	1	C	104
3.85266025	1.35611539	10.77720484	1	C	105
3.96768644	.06450537	8.66647747	1	C	106
3.76457896	-1.18808746	7.99810446	1	C	107
2.33495102	-3.19011683	7.94053376	1	C	108
.01406459	-4.01424026	7.97796916	1	C	109
-3.76362818	1.20163507	7.93854928	1	C	110
-3.77472082	-1.26644608	7.98243317	1	C	111
-2.33216050	-3.25681424	7.90674158	1	C	112

%endblock AtomicCoordinatesAndAtomicSpecies

Part of energy spectrum of the caps when they are under an external electric field 0.5 V/A

Energy unit: eV

Cap1

LUMO+2	-4.06198
LUMO+1	-4.43711

LUMO	-4.49340
HOMO	-4.77322
HOMO-1	-4.80565
HOMO-2	-4.90869

Cap2

LUMO+2	-4.34308
LUMO+1	-4.46579
LUMO	-4.48720
HOMO	-4.51082
HOMO-1	-4.84840
HOMO-2	-4.91626

Cap3

LUMO+2	-4.04414
LUMO+1	-4.53824
LUMO	-4.62279
HOMO	-4.92115
HOMO-1	-4.99250
HOMO-2	-5.02727

Cap4

LUMO+2	-4.66803
LUMO+1	-4.67128
LUMO	-4.69091
HOMO	-4.69351
HOMO-1	-5.11575
HOMO-2	-5.11934

Cap5

LUMO+2	-3.94118
LUMO+1	-4.57868
LUMO	-4.60199
HOMO	-4.90780
HOMO-1	-4.99705
HOMO-2	-5.04176

Cap6

LUMO+2	-4.32661
LUMO+1	-4.62043
LUMO	-4.63497
HOMO	-4.75229
HOMO-1	-5.05740

HOMO-2	-5.06151
