Electronic Supplementary Information (ESI) for paper: "Nanoscale Stabilization of Zintl Compounds: 1D Ionic Li-P Double Helix Confined Inside a Carbon Nanotube"

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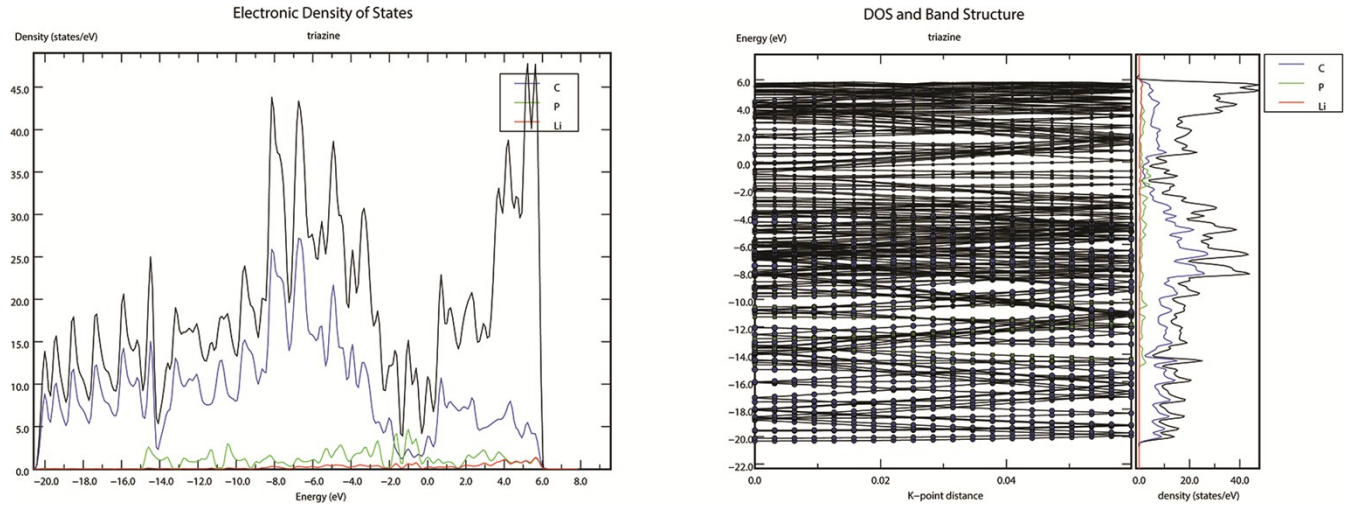

Fig. S1. Projected density of states (DOS) and band structure for LiP@SWCNT(10,0).

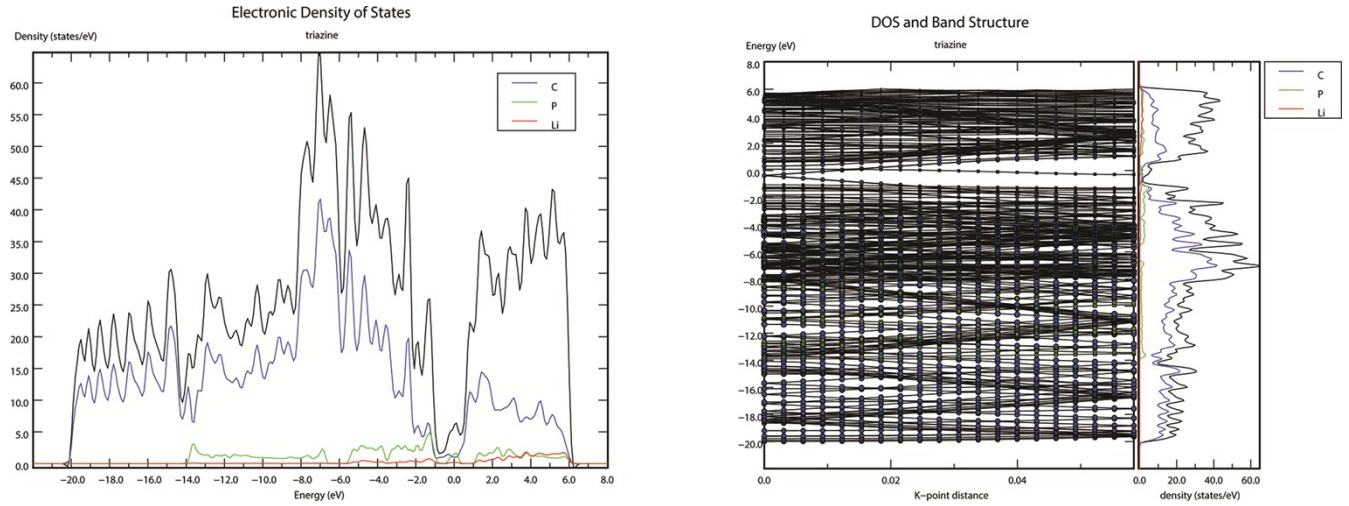

Fig. S2. Projected density of states (DOS) and band structure for LiP@SWCNT(15,0).

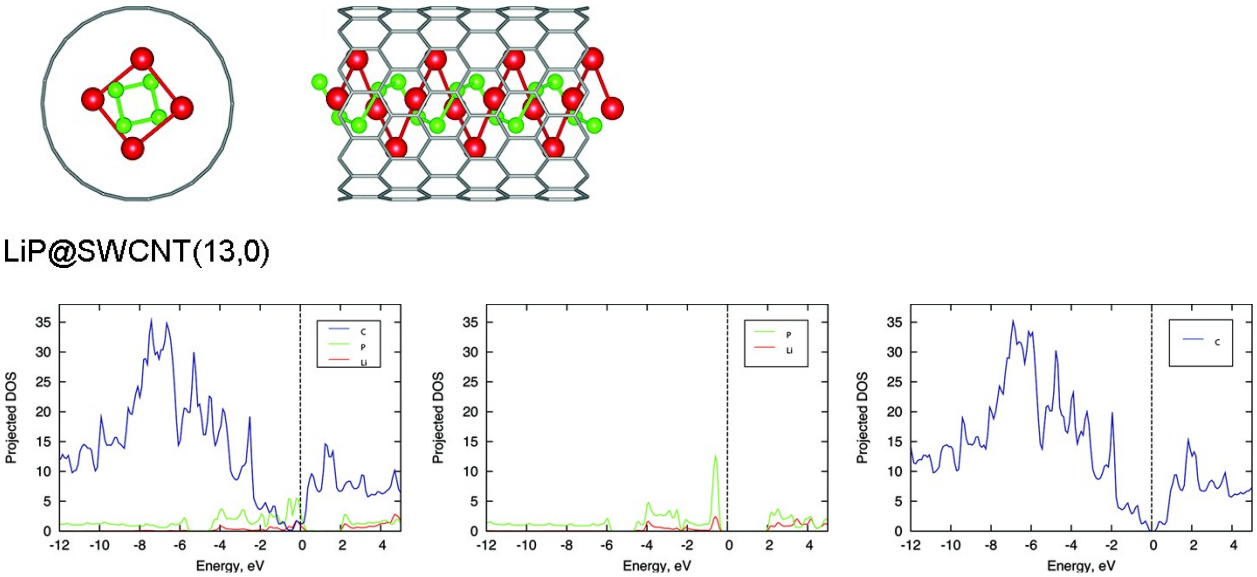

Fig. S3. End-on and side views of the fully optimized structure of LiP@SWCNT(13,0) nanocomposite as well as projected density of electronic states for the LiP@SWCNT(13,0) system (left), for the stand-alone LiP double-helical chain (center), and the carbon nanotube (right).

Table S1. P-P, Li-P, and Li-Li bond lengths (Å) in the corresponding compounds.

Compound	P-P bond length, Å	Li-P bond length, Å	Li-Li bond length, Å
LiP@SWCNT(12,0)[a]	2.19	3.69-3.70	3.49-3.59
Free standing LiP[a]	2.27	3.15	2.81
$P2_1/c$ LiP [lithium phosphide][b]	2.20-2.22	3.36-3.39	2.97-3.01
$P2_1/c$ BaP_2 [barium phosphide][c]	2.20-2.25	-	-
$P2_1/c$ SrP_2 [strontium phosphide][c]	2.20-2.25	-	-
Im-3m Li [lithium metal][d]	-	-	3.04

[a]Theoretically calculated structures obtained in this work. [b]Experimental structure [Hönle, W.; von Schnering, H.-G. *Kristallogr*. 1981, 155, 307–314]. [c]Experimental structures [Dolyniuk, J.-A.; He, H.; Ivanov, A. S.; Boldyrev, A. I.; Bobev, S.; Kovnir, K. *Inorg. Chem.* 2015, 54, 8608–8616]. [d]The closet Li-Li separation distance in the most stable form for lithium metal at 298 K [M. R. Nadler, C. P. Kempfer, *Anal. Chem*. 1959, 31, 2109]

Table S2. Calculated Bader charges for LiP@SWCNT(10,0)

Li	0.7983
Li	0.7983
Li	0.8086
Li	0.8086
Li	0.8093
Li	0.8093
Li	0.7983
Li	0.7983
P	-0.3037

P	-0.3037
P	-0.645
P	-0.645
P	-0.6547
P	-0.6547
P	-0.2959
P	-0.2959
C	-0.0734
C	-0.0734
C	0.0115
C	0.0115
C	-0.1144
C	-0.1144
C	0.0069
C	0.0069
C	-0.1014
C	-0.1014
C	0.0206
C	0.0206
C	-0.1319
C	-0.1319
C	0.0438
C	0.0438
C	-0.1176
C	-0.1176
C	0.0525
C	0.0525
C	-0.1475
C	-0.1475
C	0.0484
C	0.0484
C	-0.1129
C	-0.1129
C	0.0521
C	0.0521
C	-0.0739
C	-0.0739
C	0.0747
C	0.0747
C	-0.0893
C	-0.0893
C	0.022
C	0.022
C	-0.1082

C	-0.1082
C	-0.1458
C	-0.1458
C	-0.0939
C	-0.0939
C	0.0667
C	0.0667
C	-0.1229
C	-0.1229
C	0.0505
C	0.0505
C	-0.0806
C	-0.0806
C	-0.0064
C	-0.0064
C	-0.073
C	-0.073
C	0.052
C	0.052
C	-0.076
C	-0.076
C	-0.0189
C	-0.0189
C	-0.0925
C	-0.0925
C	-0.0004
C	-0.0004
C	-0.0727
C	-0.0726
C	0.0562
C	0.0562
C	-0.0616
C	-0.0616
C	0.0709
C	0.0709
C	-0.1362
C	-0.1362
C	0.0316
C	0.0316
C	0.0063
C	0.0063
C	0.0694
C	0.0694

Table S3. Calculated Bader charges for LiP@SWCNT(15,0)

Li	0.8437
Li	0.8543
Li	0.8477
Li	0.8558
Li	0.8375
Li	0.8488
Li	0.8422
Li	0.8369
P	-0.554
P	-0.7574
P	-0.6836
P	-0.5177
P	-0.6042
P	-0.7198
P	-0.6216
P	-0.7955
C	0.0127
C	0.0482
C	-0.0252
C	-0.0671
C	0.0696
C	0.0711
C	-0.0689
C	-0.0789
C	0.0116
C	0.0295
C	-0.0779
C	-0.0752
C	0.0259
C	0.0206
C	-0.0729
C	-0.0651
C	0.0795
C	0.0869
C	-0.0868
C	-0.1059
C	0.0532
C	0.0496
C	0.0776
C	-0.0955

C	0.0607
C	0.0645
C	0.069
C	-0.079
C	0.0574
C	0.056
C	-0.0898
C	-0.1038
C	0.04
C	0.0142
C	-0.1184
C	-0.1341
C	0.0442
C	0.0492
C	-0.0593
C	-0.0589
C	0.0666
C	0.0687
C	-0.0669
C	-0.0694
C	0.0449
C	0.0458
C	-0.0542
C	-0.0559
C	0.0449
C	0.0457
C	-0.0677
C	-0.0687
C	0.0602
C	0.0605
C	-0.0311
C	-0.033
C	-0.003
C	-0.0025
C	-0.0083
C	-0.01
C	0.0657
C	0.0694
C	-0.0718
C	-0.0748
C	0.0498
C	0.0411
C	-0.0975
C	-0.1216

C	0.0286
C	0.0361
C	-0.1391
C	-0.1159
C	0.0504
C	0.0658
C	-0.0705
C	-0.0668
C	0.0738
C	0.0276
C	-0.1033
C	-0.09
C	-0.1167
C	0.0418
C	-0.1106
C	-0.076
C	-0.0944
C	0.0621
C	-0.0955
C	-0.059
C	0.0648
C	0.0258
C	-0.092
C	-0.0845
C	0.0581
C	0.0433
C	-0.0727
C	-0.0715
C	0.0378
C	0.0363
C	-0.057
C	-0.0589
C	0.0742
C	0.0244
C	-0.0367
C	0.0101
C	0.0296
C	0.0276
C	-0.0733
C	-0.0738
C	0.0419
C	0.0401
C	-0.052
C	-0.0522

C	0.0412
C	0.0386
C	-0.0315
C	-0.0319
C	0.0237
C	0.022
C	-0.0353
C	-0.0334