Electronic Supplementary Information

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List:

S1

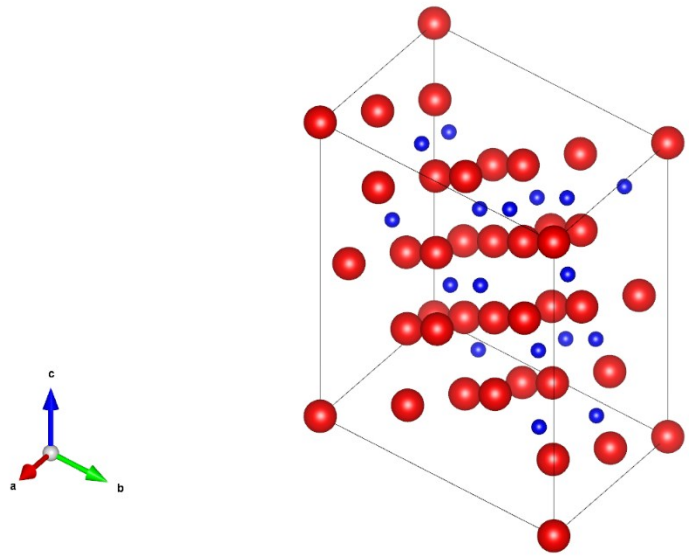

Figure S1. **$PuC_{0.347}(Pu_{32}C_{17})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T1

Table T1. **$PuC_{0.347}(Pu_{32}C_{17})$**

PuC17
1.0

9.2759428024	0.0000000000	0.0000000000
-0.6625674620	10.4970413238	0.0000000000
-3.3128364151	-4.8930433146	10.0146819134

C Pu
17 32
Cartesian

-0.662567019	2.300148487	7.041573048
-1.987701893	5.143968105	8.606367111
1.325134754	7.109549999	3.911985159
2.650270462	1.338268161	7.667490959
1.325134277	4.182088375	9.232284546
3.975404024	9.033309937	2.660149813
3.312836647	1.380089283	4.224944115
4.637971401	6.147669792	4.537902832
3.975404263	-1.505551934	6.102696896
5.300539017	3.262028694	6.415655613
3.975404263	6.105848312	7.980449677

3.312837124	-1.547372937	9.545243263
4.637972355	3.220207214	9.858201981
-0.662567317	5.227610111	1.721273422
7.288240910	8.071430206	3.286067486
-1.987701893	-2.467432499	6.728614330
0.662567317	2.383790493	0.156479403
0.000000000	0.000000000	0.000000000
-0.662567317	-0.041821122	3.442546844
-1.987701893	2.801999092	5.007340908
-1.325134635	-0.083642244	6.885093689
-2.650269270	2.760178566	8.449888229
-0.662566781	-2.969282866	8.762846947
1.325134635	4.767580986	0.312958807
0.000000094	7.611401081	1.877752662
1.987702489	1.881939650	2.190711737
0.662567437	4.725759506	3.755505323
-0.662567019	7.569581032	5.320299625
2.650269747	-1.003701210	4.068464279
1.325134397	1.840118885	5.633258343
0.000000201	4.683938980	7.198052406
1.987702489	-1.045522213	7.511010647
0.662567675	1.798297644	9.075805664
2.650269747	-3.931163311	9.388764381
2.650269270	9.535161972	0.625917614
4.637971401	3.805700541	0.938876331
3.312836885	6.649520397	2.503670454
5.300539017	0.920059443	2.816629171
3.975404978	3.763879299	4.381423473
2.650268555	6.607699394	5.946217537
5.963106155	-1.965581656	4.694382191
4.637971401	0.878238440	6.259176254
3.312837601	3.722058535	7.823970318
5.300539494	-2.007402420	8.136928558
3.975404501	0.836417437	9.701723099
5.963105202	8.573281288	1.251835227
7.950808525	2.843820333	1.564794064
6.625674725	5.687640667	3.129588127
5.963106632	5.645819664	6.572134972

S2

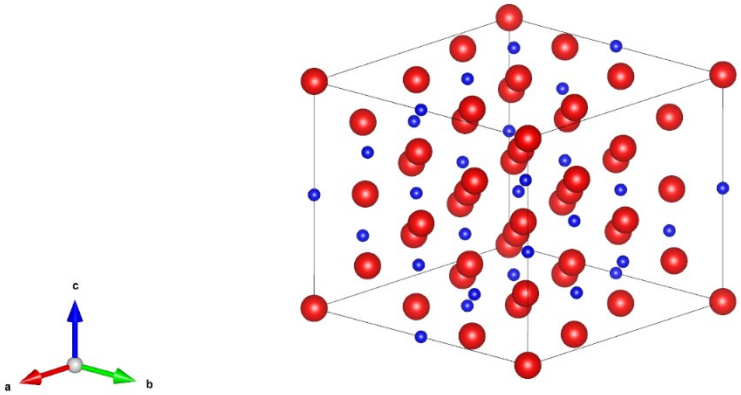

Figure S2. **$PuC_{0.36}(Pu_{32}C_{18})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T2

Table T2. **$PuC_{0.36}(Pu_{32}C_{18})$**

PuC18
1.0

11.0391426086	0.0000000000	0.0000000000
-6.6234853015	8.8313142847	0.0000000000
-2.2078280978	-4.4156560308	9.8737098622

C Pu
18 32
Cartesian

4.415657520	-2.207827568	7.405281544
4.415657043	3.311742783	0.000000000
0.000000781	5.519571781	4.936854362
1.103914857	2.207829237	4.936854362
2.207829952	4.415657997	7.405281544
-3.311742544	4.415657043	0.000000000
7.727399826	-1.103913903	2.468427181
-1.103913903	-2.207827806	4.936854362
3.311743021	1.103914618	2.468427181
5.519571781	0.000000608	4.936854362
-3.311742067	-1.103913546	7.405281544
1.103914380	2.207828522	0.000000000

-5.519570827	5.519571781	2.468427181
2.207828760	-1.103913665	4.936854362
6.623486042	2.207828760	2.468427181
-3.311742067	4.415657520	4.936854362
-2.207828283	1.103914857	4.936854362
-2.207827806	6.623486042	2.468427181
-6.623484612	3.311743736	7.405281544
-5.519570351	5.519571781	4.936854362
-4.415656567	2.207829237	4.936854362
-3.311742306	4.415657997	7.405281544
-2.207828045	1.103915215	7.405281544
-1.103913784	-2.207827568	7.405281544
-3.311742306	4.415657997	2.468427181
-2.207828045	1.103914380	2.468427181
-1.103914022	3.311743975	4.936854362
0.000000423	0.000000608	4.936854362
1.103914976	2.207829475	7.405281544
2.207828760	-1.103913546	7.405281544
-2.207828045	6.623485565	0.000000000
-1.103914022	3.311742783	0.000000000
0.000000510	5.519571781	2.468427181
0.000000000	0.000000000	0.000000000
1.103914618	2.207828760	2.468427181
2.207829237	4.415657520	4.936854362
2.207828522	-1.103913903	2.468427181
3.311743021	1.103914857	4.936854362
4.415657520	-2.207827806	4.936854362
5.519572735	0.000000740	7.405281544
6.623485088	-3.311741829	7.405281544
1.103914738	7.727399826	0.000000000
2.207828760	4.415657043	0.000000000
3.311743975	6.623486042	2.468427181
3.311742783	1.103914261	0.000000000
4.415657043	3.311743021	2.468427181
5.519571304	0.000000304	2.468427181
7.727401257	-1.103913784	4.936854362
5.519571781	5.519571781	0.000000000
6.623485565	2.207828522	0.000000000

S3

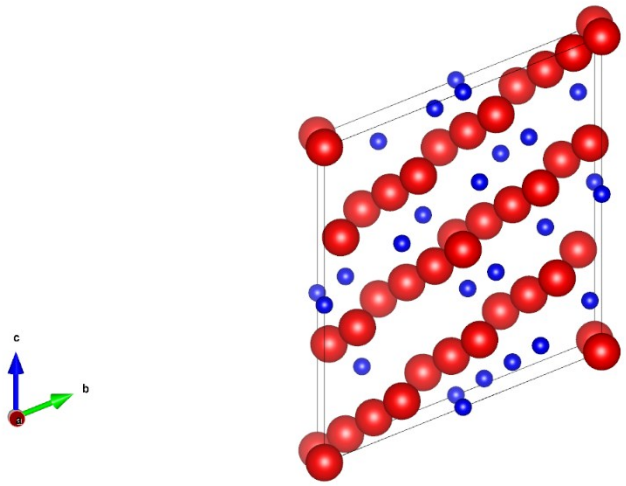

Figure S3. **$PuC_{0.373}(Pu_{32}C_{19})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T3

Table T3. **$PuC_{0.373}(Pu_{32}C_{19})$**

PuC19
1.0

9.2759428024	0.0000000000	0.0000000000
3.9754040265	10.3496326411	0.0000000000
1.3251340288	4.2416529570	10.1573191827

C Pu
19 32
Cartesian

2.650269270	2.544991732	2.221913576
10.601077080	5.429315567	6.030908108
2.650268793	6.107980251	9.205070496
4.637970924	6.532145023	6.348324299
6.625673294	6.956310749	3.491578341
9.275941849	8.313639641	9.839902878
9.938509941	8.059140205	3.808994770
11.263646126	8.737804413	6.983156681
1.987701893	5.174815655	0.000000000
5.300538540	9.840634346	7.300572872
5.300538540	6.277645111	0.317416131
7.288240433	10.264800072	4.443827629
8.613374710	10.943464279	7.617989540

8.613375664	7.380475521	0.634832442
11.926212311	8.483304024	0.952248693
0.662567019	2.120826483	5.078659534
5.963105679	13.149123192	8.252821922
3.975403309	3.223656178	5.396075726
9.275942802	10.688962936	1.587080956
0.000000000	0.000000000	0.000000000
3.312836647	1.102829695	0.317416221
4.637971401	1.781494260	3.491578341
6.625673294	2.205659389	0.634832442
7.950807571	2.884323835	3.808994770
9.275942802	3.562988520	6.983156681
9.938509941	3.308489084	0.952248693
1.987701774	3.987153292	4.126410961
3.312835932	4.665818214	7.300572872
3.975404024	4.411318779	1.269664884
5.300538540	5.089983463	4.443827152
6.625673294	5.768647671	7.617989540
7.288239956	5.514148712	1.587080956
8.613374710	6.192813396	4.761243343
9.938509941	6.871477604	7.935405731
10.601078033	6.616978168	1.904497504
2.650269032	7.295642853	5.078659534
3.975403547	7.974306583	8.252821922
4.637971401	7.719808102	2.221913338
5.963105679	8.398471832	5.396075726
7.288240433	9.077136993	8.570238113
7.950808048	8.822637558	2.539329767
9.275942802	9.501301765	5.713491917
10.601077080	10.179966927	8.887654305
11.263645172	9.925466537	2.856745958
12.588779449	10.604131699	6.030908108
4.637970924	11.282795906	9.205070496
5.300538540	11.028296471	3.174162626
6.625673294	11.706961632	6.348324299
7.950807571	12.385626793	9.522486687
9.938509941	12.809790611	6.665740490
11.263644218	13.488455772	9.839902878

S4

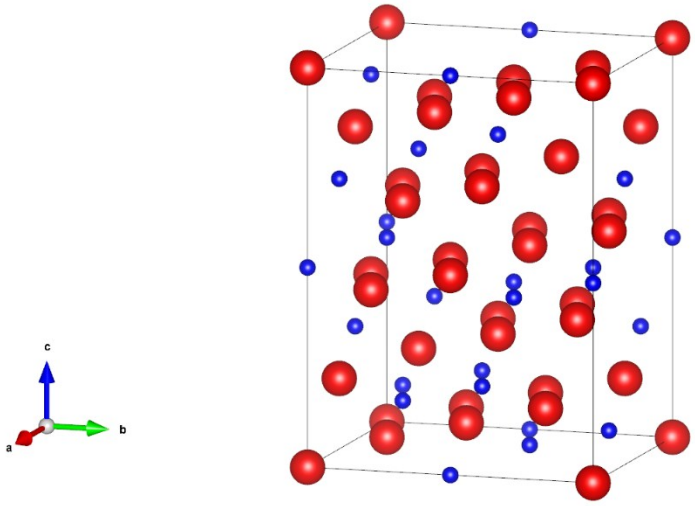

Figure S4. **$PuC_{0.385}(Pu_{32}C_{20})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T4

Table T4. **$PuC_{0.385}(Pu_{32}C_{20})$**

PuC20
1.0

6.0725297928	0.0000000000	0.0000000000
-2.0241770949	10.9005247612	0.0000000000
-2.0241767683	-0.3758802755	14.7314344108

C Pu
20 32
Cartesian

1.012088180	4.698502064	2.762144327
-1.012088537	5.450262547	0.000000000
-0.000000186	5.638202667	5.984645367
4.048352718	6.389962673	3.222501516
2.024176121	7.141723156	0.460357338
3.036264420	7.329663277	6.445002556
-2.024177074	9.772884369	4.143216133
2.024176121	10.524644852	1.381072283
1.012088180	1.315580606	1.841429353
1.012087703	5.826143265	11.969290733
-1.012088776	9.960824013	10.127861023
-0.000000261	9.021123886	6.905360699
-1.012088418	-0.187940136	7.365717411

3.036264658	0.563820243	4.603573322
-0.000000112	2.255280972	5.063930511
4.048353672	3.007041454	2.301786661
-0.000000425	-0.000000087	13.350362778
4.048353672	0.751760304	10.588218689
2.024176359	1.503520966	7.826074600
1.012087703	2.443221092	11.048577309
5.060441494	0.939700425	3.222501278
0.000000000	0.000000000	0.000000000
3.036264658	1.691460729	0.460357338
1.012087941	0.187940046	5.984645367
4.048353672	1.879400849	6.445002556
2.024176359	2.631161213	3.682858706
-0.000000164	3.382921457	0.920714676
3.036264658	5.074382305	1.381072164
2.024175882	0.375880092	11.969290733
-0.000000030	1.127640605	9.207146645
3.036264420	2.819101572	9.667505264
1.012088180	3.570861578	6.905360699
-1.012088537	4.322622299	4.143216133
2.024176121	6.014082909	4.603573322
-0.000000328	6.765842915	1.841429353
3.036264181	8.457304955	2.301786900
-1.012088776	2.067340851	12.429649353
2.024176598	3.758801699	12.890005112
-0.000000224	4.510561943	10.127861023
3.036264181	6.202022552	10.588218689
-2.024177074	5.262322426	7.365717411
1.012087703	6.953783035	7.826074600
-1.012088537	7.705543518	5.063930511
2.024176359	9.397004128	5.524288654
-0.000000403	10.148764610	2.762144327
-1.012088895	5.450262547	13.350362778
2.024176359	7.141723156	13.810721397
-0.000000657	7.893483639	11.048577309
-2.024177074	8.645244598	8.286432266
1.012088060	10.336705208	8.746788979
-1.012088776	8.833185196	14.271077156
-3.036265612	9.584944725	11.508933067

S5

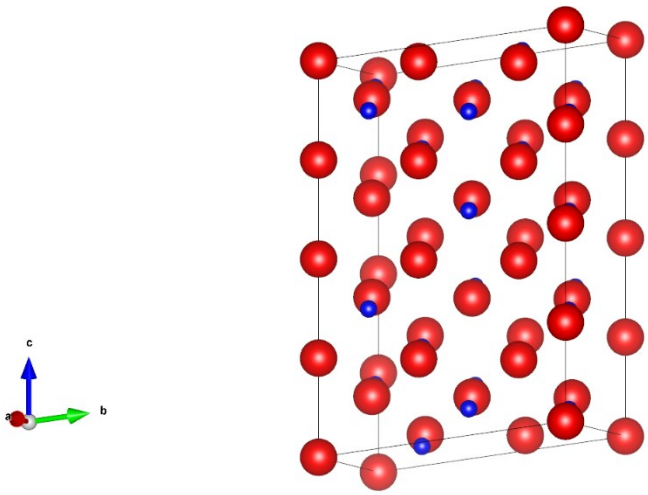

Figure S5. **$PuC_{0.396}(Pu_{32}C_{21})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T5

Table T5. **$PuC_{0.396}(Pu_{32}C_{21})$**

PuC21
1.0

7.8396024704	0.0000000000	0.0000000000
0.7839601338	9.2427550753	0.0000000000
3.1358412560	2.3938071035	13.4575693669

C Pu
21 32
Cartesian

4.703760624	2.925764322	0.210274518
6.271681786	8.777291298	0.630823672
7.055641651	4.721119404	10.303451538
8.623562813	10.572648048	10.723999977
4.703761578	6.250496387	12.406196594
5.487721920	2.859269619	12.826745987
7.055642605	8.710798264	13.247295380
7.839602470	9.974196434	7.359608173
6.271682262	8.112345695	9.882902145
10.191483498	3.790194511	11.565098763
3.919801474	9.641723633	11.985646248
5.487720966	3.524215937	3.574666739
7.055642128	9.375744820	3.995215893

3.135840893	5.053592682	5.677412033
9.407523155	7.181420326	11.144549370
2.351880550	4.455141068	2.313019753
3.135840654	1.063914299	2.733568430
8.623562813	2.593291044	4.836313725
2.351880789	8.444819450	5.256863117
8.623562813	6.582969189	7.780157089
7.055642128	5.386065006	1.051372528
9.407523155	9.176259995	12.616471291
10.191483498	5.785034180	13.037019730
8.623562813	8.577808380	9.252079010
9.407523155	5.186582088	9.672627449
6.271681786	10.107185364	11.354824066
7.055642605	6.715958118	11.775373459
7.839602470	3.324732065	12.195921898
7.839602470	7.979356766	5.887686729
8.623562813	4.588130474	6.308235645
5.487721443	9.508733749	7.990431786
6.271682739	6.117506981	8.410980225
7.055642128	2.726280212	8.831529617
3.919801235	7.646883965	10.513726234
4.703762054	4.255656719	10.934273720
7.055642128	7.380904198	2.523294210
7.839602470	3.989678383	2.943843365
4.703761101	8.910282135	4.626039505
5.487721920	5.519055367	5.046588421
6.271681309	2.127828598	5.467136860
3.135841370	7.048431873	7.149333477
3.919801712	3.657205582	7.569882393
2.351881027	1.795355320	10.093176842
3.919800997	8.311830521	1.261647224
4.703761578	4.920602798	1.682196140
5.487720966	1.529376745	2.102745056
2.351880550	6.449980259	3.784941196
3.135841370	3.058753490	4.205490112
1.567920685	1.196903586	6.728784561
1.567920446	5.851528645	0.420549035
2.351880789	2.460301399	0.841098070
0.783960342	0.598451793	3.364392281
0.000000000	0.000000000	0.000000000

S6

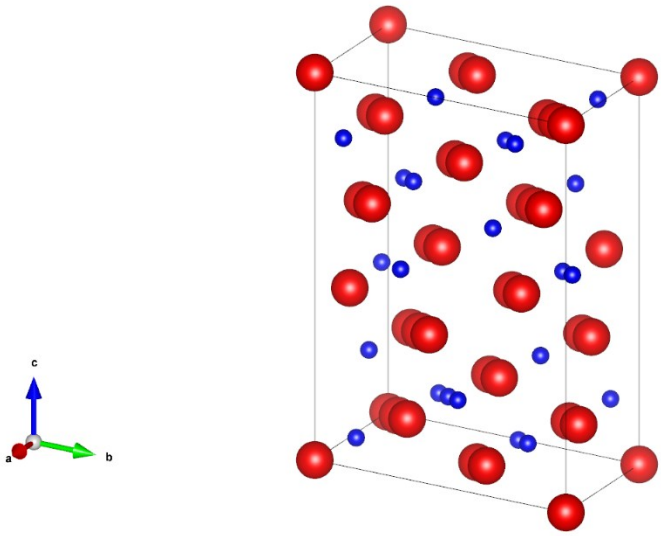

Figure S6. **$PuC_{0.407}(Pu_{32}C_{22})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T6

Table T6. **$PuC_{0.407}(Pu_{32}C_{22})$**

PuC22
1.0

7.8396024704	0.0000000000	0.0000000000
0.0000000000	9.2759428024	0.0000000000
-0.7839604133	-1.9877015785	13.4094207768

C Pu
22 32
Cartesian

2.351880789	5.963106155	3.771399736
5.487722397	4.637971878	8.799932480
7.055643082	4.637971401	2.933310986
3.135840893	3.975404739	11.314198494
1.567920446	5.300538540	0.419044405
5.487722397	1.987702489	12.990376472
3.919801235	3.312836885	2.095221996
7.055642128	1.987702489	7.123754978
4.703761578	1.325135350	9.638021469
0.783960223	1.987702131	1.257133245
1.567920327	0.000000160	8.799932480
7.055642128	-0.662566781	11.314198494
5.487720966	0.662567377	0.419044405

3.135840893	0.000000093	2.933310747
0.783960104	-0.662567139	5.447577477
6.271681786	7.950808525	7.961843491
0.000000054	7.950808525	2.095222235
4.703761578	6.625673294	1.257133365
1.567920685	6.625674248	12.990376472
3.135840893	6.625673771	7.123754978
0.783960104	5.963106632	9.638021469
6.271681786	5.300539970	12.152287483
5.487720966	8.613375664	2.514266491
3.135840893	7.950808525	5.028532982
0.783960164	7.288241386	7.542799473
2.351880789	7.288240910	1.676177859
0.000000041	6.625673771	4.190443993
6.271681786	6.625674248	10.057065964
3.919801235	5.963106632	12.571331978
5.487721443	5.963106155	6.704710484
3.135840893	5.300539017	9.218976974
0.783960044	4.637971878	11.733242989
7.055642128	5.963106155	0.838088930
4.703761578	5.300539017	3.352355242
2.351880312	4.637971878	5.866621494
-0.000000037	3.975404263	8.380887985
3.919801235	4.637971401	0.000000000
1.567920446	3.975404263	2.514266491
5.487722397	3.312836885	10.895154953
7.055642128	3.312837124	5.028532982
4.703761578	2.650269985	7.542799473
2.351880550	1.987702250	10.057065964
-0.000000115	1.325135350	12.571331978
6.271681786	2.650269508	1.676177621
3.919800997	1.987702131	4.190443993
1.567920446	1.325134993	6.704710484
3.135840893	1.325134754	0.838088810
0.783960223	0.662567496	3.352355242
0.000000000	0.000000000	0.000000000
7.055642128	0.662567794	9.218976974
4.703760624	0.000000611	11.733242989
6.271681786	0.000000186	5.866621494
3.919800997	-0.662567079	8.380887985
1.567920208	-1.325134277	10.895154953

S7

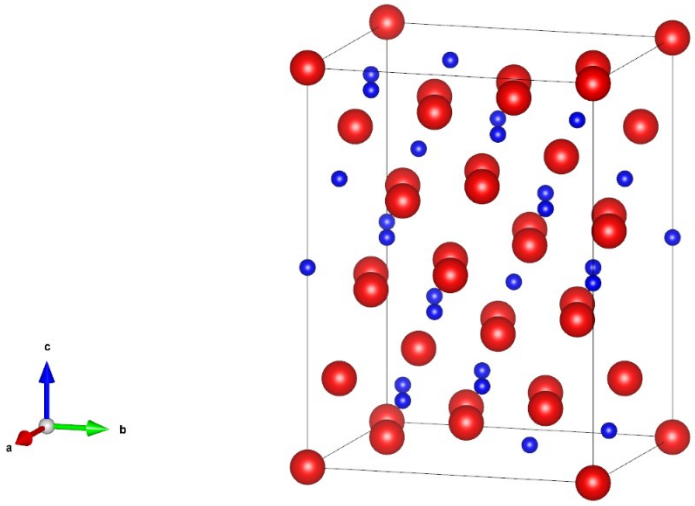

Figure S7. **$PuC_{0.418}(Pu_{32}C_{23})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T7

Table T7. **$PuC_{0.418}(Pu_{32}C_{23})$**

PuC23
1.0

6.0725297928	0.0000000000	0.0000000000
-2.0241770949	10.9005247612	0.0000000000
-2.0241767683	-0.3758802755	14.7314344108

C Pu
23 32
Cartesian

1.012088180	4.698502064	2.762144327
-0.000000380	3.382921457	14.271077156
3.036264896	3.946741819	5.524288654
-0.000000186	5.638202667	5.984645367
4.048352718	6.389962673	3.222501516
2.024176121	7.141723156	0.460357338
-2.024177074	4.134682178	11.508933067
-1.012088776	6.577902794	9.207146645
2.024176121	10.524644852	1.381072283
1.012088180	1.315580606	1.841429353
1.012087703	5.826143265	11.969290733
2.024175882	8.269363403	9.667505264
-1.012088776	9.960824013	10.127861023

-0.000000261	9.021123886	6.905360699
-1.012088418	-0.187940136	7.365717411
-0.000000112	2.255280972	5.063930511
4.048353672	3.007041454	2.301786661
1.012087941	9.209063530	12.890005112
-0.000000425	-0.000000087	13.350362778
4.048353672	0.751760304	10.588218689
2.024176359	1.503520966	7.826074600
3.036264420	1.691460729	13.810721397
1.012087703	2.443221092	11.048577309
5.060441494	0.939700425	3.222501278
0.000000000	0.000000000	0.000000000
3.036264658	1.691460729	0.460357338
1.012087941	0.187940046	5.984645367
4.048353672	1.879400849	6.445002556
2.024176359	2.631161213	3.682858706
-0.000000164	3.382921457	0.920714676
3.036264658	5.074382305	1.381072164
2.024175882	0.375880092	11.969290733
-0.000000030	1.127640605	9.207146645
3.036264420	2.819101572	9.667505264
1.012088180	3.570861578	6.905360699
-1.012088537	4.322622299	4.143216133
2.024176121	6.014082909	4.603573322
-0.000000328	6.765842915	1.841429353
3.036264181	8.457304955	2.301786900
-1.012088776	2.067340851	12.429649353
2.024176598	3.758801699	12.890005112
-0.000000224	4.510561943	10.127861023
3.036264181	6.202022552	10.588218689
-2.024177074	5.262322426	7.365717411
1.012087703	6.953783035	7.826074600
-1.012088537	7.705543518	5.063930511
2.024176359	9.397004128	5.524288654
-0.000000403	10.148764610	2.762144327
-1.012088895	5.450262547	13.350362778
2.024176359	7.141723156	13.810721397
-0.000000657	7.893483639	11.048577309
-2.024177074	8.645244598	8.286432266
1.012088060	10.336705208	8.746788979
-1.012088776	8.833185196	14.271077156
-3.036265612	9.584944725	11.508933067

S8

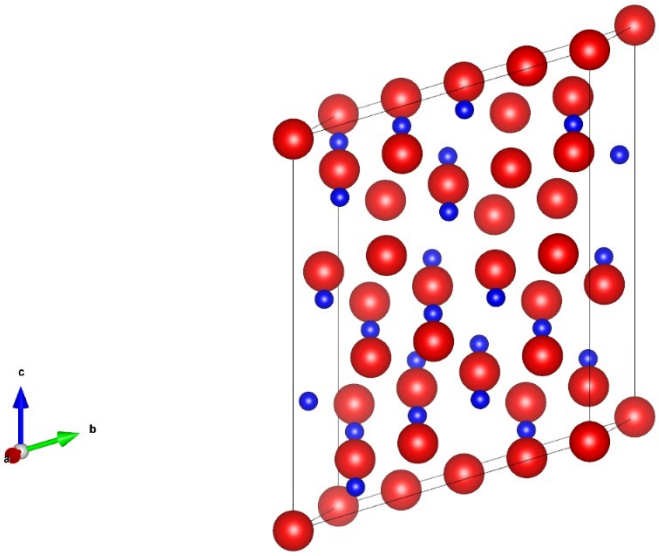

Figure S8. **$PuC_{0.428}(Pu_{32}C_{24})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T8

Table T8. **$PuC_{0.428}(Pu_{32}C_{24})$**

PuC24
1.0

7.8396024704	0.0000000000	0.0000000000
1.5679205520	10.4004085178	0.0000000000
0.7839609206	4.0183395225	11.9596278417

C Pu
24 32
Cartesian

6.271683216	1.418237567	3.737383842
0.783960462	4.018339634	3.737383842
7.055642605	3.072847843	6.727290630
3.135840893	6.618442059	3.737383842
8.623563766	8.745798111	5.232337475
3.919801950	3.545593739	5.232337475
1.567921042	5.672950268	6.727290630
7.839602947	4.727458954	9.717197418
5.487721920	9.218544006	3.737383842
3.135841370	11.345900536	5.232337475
6.271682262	6.145696640	5.232337475
2.351881504	7.327560902	9.717197418

7.839603901	9.454916954	11.212152481
3.135842085	4.254712582	11.212152481
7.839602470	2.363729239	0.747476697
3.919801712	13.000511169	8.222244263
7.055642605	7.800306320	8.222244263
5.487722397	6.854815483	11.212152481
7.839602470	7.091187477	2.242430210
3.135841131	1.890983582	2.242430210
7.055642605	12.527766228	9.717197418
4.703761101	7.563934326	0.747476816
2.351881027	9.691289902	2.242430210
5.487721920	4.491085529	2.242430210
0.000000000	0.000000000	0.000000000
2.351880789	2.600102186	0.000000000
0.783960462	1.654610395	2.989907026
4.703761578	5.200204372	0.000000000
2.351880789	7.327561378	1.494953513
5.487721920	2.127356291	1.494953513
3.135841608	4.254712582	2.989907026
1.567920923	3.309220791	5.979814053
7.055642128	7.800307274	0.000000000
4.703762531	9.927662849	1.494953513
7.839602470	4.727458477	1.494953394
5.487720966	6.854814529	2.989907026
3.135841370	8.982171059	4.484860420
6.271682262	3.781967163	4.484860420
3.919801474	5.909323692	5.979814053
1.567920923	8.036679268	7.474767685
4.703761101	2.836474895	7.474767685
2.351881266	4.963831425	8.969720840
7.839601994	9.454916954	2.989907026
5.487722397	11.582272530	4.484860420
8.623562813	6.382069111	4.484860420
6.271683216	8.509425163	5.979814053
3.919801712	10.636781693	7.474767685
7.055642605	5.436577320	7.474767685
4.703762054	7.563933849	8.969720840
2.351881504	9.691289902	10.464674950
5.487723351	4.491085529	10.464674950
8.623561859	11.109527588	5.979814053
7.055643082	10.164035797	8.969720840
4.703762531	12.291393280	10.464674950
7.839603901	7.091187477	10.464674950
9.407524109	12.764138222	8.969720840

S9

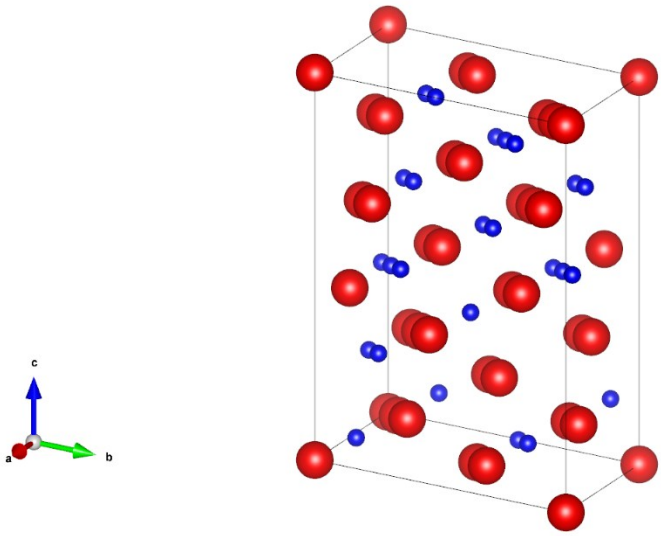

Figure S9. **$PuC_{0.438}(Pu_{32}C_{25})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T9

Table T9. **$PuC_{0.438}(Pu_{32}C_{25})$**

PuC25
1.0

7.8396024704	0.0000000000	0.0000000000
0.0000000000	9.2759428024	0.0000000000
-0.7839604133	-1.9877015785	13.4094207768

C Pu
25 32
Cartesian

0.000000002	5.300539017	6.285665989
5.487722397	4.637971878	8.799932480
4.703761578	3.975404263	5.447577477
3.135840893	3.975404739	11.314198494
1.567920446	5.300538540	0.419044405
2.351880550	3.312837124	7.961843491
0.000000026	2.650269747	10.476110458
5.487722397	1.987702489	12.990376472
7.055642128	1.987702489	7.123754978
4.703761578	1.325135350	9.638021469
0.783960223	1.987702131	1.257133245
6.271681786	1.325134993	3.771399736
2.351881027	0.662567973	12.152287483

3.919800997	0.662567556	6.285665989
1.567920327	0.000000160	8.799932480
5.487720966	0.662567377	0.419044405
3.135840893	0.000000093	2.933310747
0.783960104	-0.662567139	5.447577477
6.271681786	7.950808525	7.961843491
0.000000054	7.950808525	2.095222235
4.703761578	6.625673294	1.257133365
3.919800758	7.288241386	10.476110458
3.135840893	6.625673771	7.123754978
0.783960104	5.963106632	9.638021469
6.271681786	5.300539970	12.152287483
5.487720966	8.613375664	2.514266491
3.135840893	7.950808525	5.028532982
0.783960164	7.288241386	7.542799473
2.351880789	7.288240910	1.676177859
0.000000041	6.625673771	4.190443993
6.271681786	6.625674248	10.057065964
3.919801235	5.963106632	12.571331978
5.487721443	5.963106155	6.704710484
3.135840893	5.300539017	9.218976974
0.783960044	4.637971878	11.733242989
7.055642128	5.963106155	0.838088930
4.703761578	5.300539017	3.352355242
2.351880312	4.637971878	5.866621494
-0.000000037	3.975404263	8.380887985
3.919801235	4.637971401	0.000000000
1.567920446	3.975404263	2.514266491
5.487722397	3.312836885	10.895154953
7.055642128	3.312837124	5.028532982
4.703761578	2.650269985	7.542799473
2.351880550	1.987702250	10.057065964
-0.000000115	1.325135350	12.571331978
6.271681786	2.650269508	1.676177621
3.919800997	1.987702131	4.190443993
1.567920446	1.325134993	6.704710484
3.135840893	1.325134754	0.838088810
0.783960223	0.662567496	3.352355242
0.000000000	0.000000000	0.000000000
7.055642128	0.662567794	9.218976974
4.703760624	0.000000611	11.733242989
6.271681786	0.000000186	5.866621494
3.919800997	-0.662567079	8.380887985
1.567920208	-1.325134277	10.895154953

S10

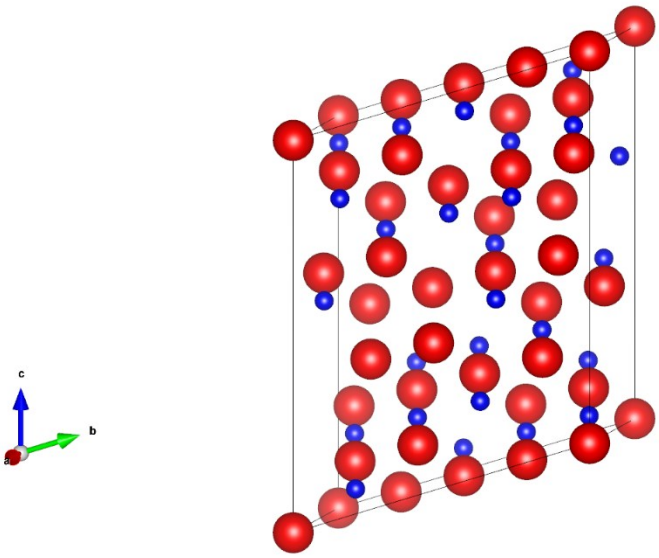

Figure S10. **$PuC_{0.448}(Pu_{32}C_{26})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T10

Table T10. **$PuC_{0.448}(Pu_{32}C_{26})$**

PuC26
1.0

7.8396024704	0.0000000000	0.0000000000
1.5679205520	10.4004085178	0.0000000000
0.7839609206	4.0183395225	11.9596278417

C Pu
26 32
Cartesian

0.783960462	4.018339634	3.737383842
7.055642605	3.072847843	6.727290630
3.135840893	6.618442059	3.737383842
8.623563766	8.745798111	5.232337475
7.839602947	4.727458954	9.717197418
5.487721920	9.218544006	3.737383842
3.135841370	11.345900536	5.232337475
3.919801712	8.273052216	6.727290630
9.407524109	10.400408745	8.222244263
4.703762054	5.200204372	8.222244263
7.839603901	9.454916954	11.212152481
3.135842085	4.254712582	11.212152481
7.839602470	2.363729239	0.747476697

3.919801712	13.000511169	8.222244263
7.055642605	7.800306320	8.222244263
4.703762054	9.927663803	9.717197418
2.351881504	12.055020332	11.212152481
5.487722397	6.854815483	11.212152481
2.351881266	4.963831425	0.747476757
7.839602470	7.091187477	2.242430210
3.135841131	1.890983582	2.242430210
7.055642605	12.527766228	9.717197418
4.703761101	7.563934326	0.747476816
2.351881027	9.691289902	2.242430210
5.487721920	4.491085529	2.242430210
7.055642128	10.164035797	0.747476697
0.000000000	0.000000000	0.000000000
2.351880789	2.600102186	0.000000000
0.783960462	1.654610395	2.989907026
4.703761578	5.200204372	0.000000000
2.351880789	7.327561378	1.494953513
5.487721920	2.127356291	1.494953513
3.135841608	4.254712582	2.989907026
1.567920923	3.309220791	5.979814053
7.055642128	7.800307274	0.000000000
4.703762531	9.927662849	1.494953513
7.839602470	4.727458477	1.494953394
5.487720966	6.854814529	2.989907026
3.135841370	8.982171059	4.484860420
6.271682262	3.781967163	4.484860420
3.919801474	5.909323692	5.979814053
1.567920923	8.036679268	7.474767685
4.703761101	2.836474895	7.474767685
2.351881266	4.963831425	8.969720840
7.839601994	9.454916954	2.989907026
5.487722397	11.582272530	4.484860420
8.623562813	6.382069111	4.484860420
6.271683216	8.509425163	5.979814053
3.919801712	10.636781693	7.474767685
7.055642605	5.436577320	7.474767685
4.703762054	7.563933849	8.969720840
2.351881504	9.691289902	10.464674950
5.487723351	4.491085529	10.464674950
8.623561859	11.109527588	5.979814053
7.055643082	10.164035797	8.969720840
4.703762531	12.291393280	10.464674950
7.839603901	7.091187477	10.464674950

9.407524109 12.764138222 8.969720840

S11

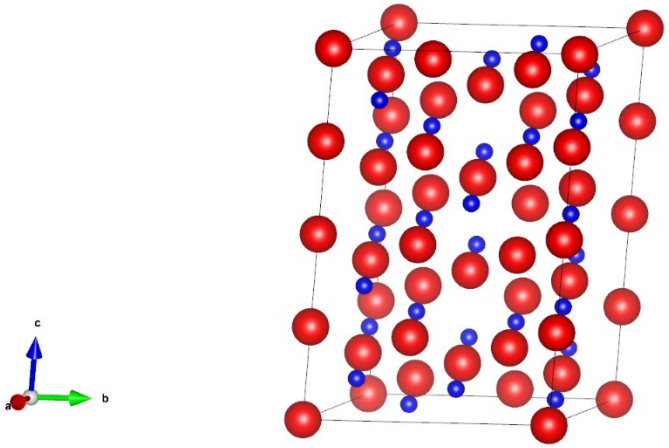

Figure S11. **$PuC_{0.458}(Pu_{32}C_{27})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T11

Table T11. **$PuC_{0.458}(Pu_{32}C_{27})$**

PuC27
1.0

7.8396024704	0.0000000000	0.0000000000
0.7839601338	9.2427550753	0.0000000000
3.1358412560	2.3938071035	13.4575693669

C Pu
27 32
Cartesian

4.703760624	2.925764322	0.210274518
6.271681786	8.777291298	0.630823672
7.055641651	4.721119404	10.303451538
8.623562813	10.572648048	10.723999977
4.703761578	6.250496387	12.406196594
5.487721920	2.859269619	12.826745987
7.055642605	8.710798264	13.247295380
6.271681309	4.122668266	6.939059258
7.839602470	9.974196434	7.359608173
3.919801235	5.652044773	9.041804314
4.703761578	2.260817766	9.462353706
6.271682262	8.112345695	9.882902145

10.191483498	3.790194511	11.565098763
3.919801474	9.641723633	11.985646248
5.487720966	3.524215937	3.574666739
7.055642128	9.375744820	3.995215893
3.135840893	5.053592682	5.677412033
3.919801235	1.662366033	6.097960949
2.351880550	4.455141068	2.313019753
3.135840654	1.063914299	2.733568430
4.703761578	6.915442467	3.154118061
8.623562813	2.593291044	4.836313725
2.351880789	8.444819450	5.256863117
8.623562813	6.582969189	7.780157089
7.839603424	1.994839191	1.471921563
1.567920208	7.846367836	1.892470837
7.055642128	5.386065006	1.051372528
9.407523155	9.176259995	12.616471291
10.191483498	5.785034180	13.037019730
8.623562813	8.577808380	9.252079010
9.407523155	5.186582088	9.672627449
6.271681786	10.107185364	11.354824066
7.055642605	6.715958118	11.775373459
7.839602470	3.324732065	12.195921898
7.839602470	7.979356766	5.887686729
8.623562813	4.588130474	6.308235645
5.487721443	9.508733749	7.990431786
6.271682739	6.117506981	8.410980225
7.055642128	2.726280212	8.831529617
3.919801235	7.646883965	10.513726234
4.703762054	4.255656719	10.934273720
7.055642128	7.380904198	2.523294210
7.839602470	3.989678383	2.943843365
4.703761101	8.910282135	4.626039505
5.487721920	5.519055367	5.046588421
6.271681309	2.127828598	5.467136860
3.135841370	7.048431873	7.149333477
3.919801712	3.657205582	7.569882393
2.351881027	1.795355320	10.093176842
3.919800997	8.311830521	1.261647224
4.703761578	4.920602798	1.682196140
5.487720966	1.529376745	2.102745056
2.351880550	6.449980259	3.784941196
3.135841370	3.058753490	4.205490112
1.567920685	1.196903586	6.728784561
1.567920446	5.851528645	0.420549035

2.351880789	2.460301399	0.841098070
0.783960342	0.598451793	3.364392281
0.000000000	0.000000000	0.000000000

S12

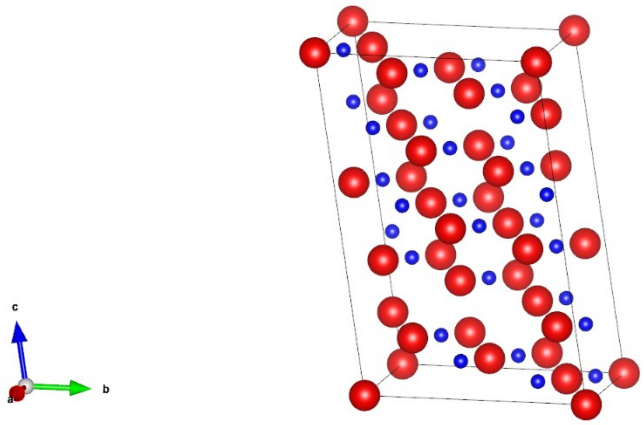

Figure S12. **$PuC_{0.467}(Pu_{32}C_{28})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T12

Table T12. **$PuC_{0.467}(Pu_{32}C_{28})$**

PuC28
1.0

7.8396024704	0.0000000000	0.0000000000
-2.3518806930	8.9728352309	0.0000000000
-2.3518812523	-3.3562508899	13.8623984449

C Pu
28 32
Cartesian

0.783959746	5.000130653	8.880599022
-0.000000571	3.424746752	11.912997246
4.703761578	6.712502956	0.649799883
1.567920446	5.205614567	1.082999706
-1.567920804	5.068625450	6.281399250
0.783959746	3.630231380	4.115399361
3.135839939	3.561736345	6.714599133
-2.351881504	3.493242264	9.313798904
-0.000000570	2.054847956	7.147799015

2.351880550	1.986353159	9.746998787
-3.135841370	1.917858720	12.346197128
-0.783960640	0.479464889	10.180198669
1.567920446	0.410970241	12.779397011
6.271682739	3.698725939	1.516199827
3.135840893	2.191837788	1.949399710
2.351881027	0.616454661	4.981799126
4.703761101	0.547959745	7.580998898
1.567920208	-0.958928585	8.014199257
3.919800758	-1.027423739	10.613398552
0.783959508	-2.534312248	11.046598434
3.135840416	-2.602806568	13.645797729
-0.000000369	8.219390869	0.216599911
2.351880550	8.150896072	2.815799713
-0.783960462	-0.890433908	5.414999485
-0.783960700	6.644008636	3.248999596
1.567920208	6.575513840	5.848199368
3.919800997	6.507018089	8.447399139
3.135839701	4.931634903	11.479798317
-0.783960581	7.328958511	5.631599426
-1.567920804	5.753574371	8.663997650
0.783959806	5.685079098	11.263198853
-2.351881504	4.178191662	11.696398735
2.351880550	7.465947151	0.433199853
4.703761578	7.397451878	3.032399654
-0.783960402	5.959058285	0.866399884
1.567920446	5.890563965	3.465599537
3.919800520	5.822069645	6.064799309
-1.567920804	4.383675575	3.898799419
0.783959925	4.315180779	6.497999191
3.135841131	4.246685505	9.097197533
-2.351881027	2.808292389	6.931199074
-0.000000381	2.739797831	9.530398369
2.351880074	2.671302557	12.129598618
-0.783960998	1.164414048	12.562798500
3.919800997	4.452170372	1.299599886
0.783960223	2.945281982	1.732799768
3.135840893	2.876787186	4.331998825
-0.000000191	1.369898915	4.765199184
2.351879835	1.301403761	7.364398956
4.703762054	1.232909322	9.963598251
-0.783960521	-0.205484524	7.797598839
1.567919970	-0.273979366	10.396799088
3.919800043	-0.342474222	12.995998383

-1.567920923	-1.780867815	10.829998970
0.783959329	-1.849362612	13.429198265
5.487722397	1.438393593	2.165999413
0.000000000	0.000000000	0.000000000
2.351880550	-0.068494841	2.599199772
4.703761101	-0.136989683	5.198399544
3.919800282	-1.712372899	8.230798721

S13

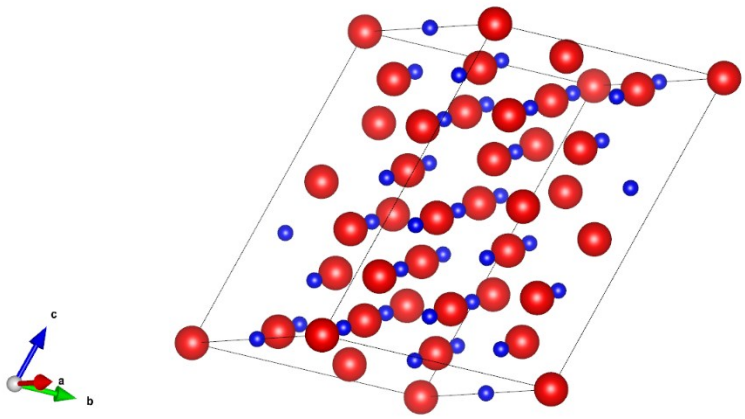

Figure S13. **$PuC_{0.475}(Pu_{32}C_{29})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T13

Table T13. **$PuC_{0.475}(Pu_{32}C_{29})$**

PuC29
1.0

8.5878543854	0.0000000000	0.0000000000
2.8626176276	8.8231816933	0.0000000000
2.8626188683	3.2506454900	12.8692204183

C Pu
29 32
Cartesian

1.431309223	3.715024471	1.608652592
4.293927193	6.269102573	8.445425987
10.019164085	6.501291752	10.456241608
4.293927670	4.875968456	11.662731171

7.156546116	6.733480453	12.467057228
7.156545162	1.857512116	0.804326296
4.293926716	9.055372238	2.010815620
10.019162178	5.804724693	4.423795223
7.156545639	6.036913872	6.434610367
7.156545162	4.643779755	9.651915550
10.019164085	3.018456459	10.858406067
4.293927193	0.000000000	0.000000000
10.019164085	7.197859764	1.206489682
7.156545162	3.947212696	3.619468212
1.431309342	2.321889877	4.825957775
4.293927193	4.179401875	5.630284309
7.156545639	2.554078817	6.836773396
4.293927670	9.751937866	8.043262482
10.019164085	9.984127045	10.054079056
4.293927670	8.358803749	11.260568619
7.156546116	10.216316223	12.064895630
7.156545162	5.340346813	0.402163029
4.293927193	2.089700937	2.815142155
10.019163132	9.287559509	4.021631241
4.293927193	7.662236691	5.228120804
7.156545162	9.519748688	6.032447815
7.156545639	8.126614571	9.249752045
7.156545639	7.430048466	3.217305183
4.293927193	5.572535992	2.412978888
11.450473785	10.216316223	12.064895630
11.450471878	9.519748688	6.032447815
8.587854385	9.751937866	8.043262482
11.450473785	8.126614571	9.249752045
5.725236416	9.984127045	10.054079056
8.587854385	8.358803749	11.260568619
11.450473785	6.733480930	12.467058182
8.587854385	9.055372238	2.010815859
5.725236416	9.287559509	4.021631241
8.587854385	7.662236691	5.228120804
5.725236893	7.894425392	7.238936424
8.587854385	6.269102573	8.445425987
5.725236416	6.501291752	10.456241608
8.587856293	4.875968456	11.662731171
5.725235939	7.197859764	1.206489325
8.587854385	5.572535992	2.412978888
2.862617970	7.430048466	3.217305183
5.725236893	5.804724693	4.423795223
8.587854385	4.179401875	5.630284309

2.862618446	6.036913872	6.434610367
5.725236416	4.411590576	7.641099930
8.587855339	2.786267519	8.847590446
2.862618685	4.643779755	9.651915550
5.725236893	3.018456459	10.858406067
2.862617970	5.340346813	0.402163148
5.725235462	3.715024233	1.608652592
8.587856293	2.089700937	2.815142155
2.862618446	3.947212696	3.619468212
5.725236416	2.321889877	4.825957775
2.862618685	2.554078817	6.836773396
2.862617731	1.857512116	0.804326296
0.000000000	0.000000000	0.000000000

S14

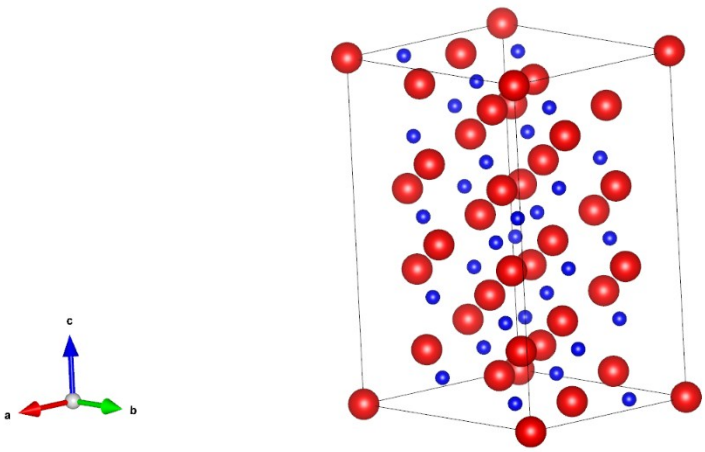

Figure S14. **$PuC_{0.484}(Pu_{32}C_{30})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T14

Table T14. **$PuC_{0.484}(Pu_{32}C_{30})$**

PuC30
1.0

7.8396024704	0.0000000000	0.0000000000
-2.3518806930	8.9728352309	0.0000000000
-2.3518812523	-3.3562508899	13.8623984449

C Pu
30 32

Cartesian

0.783959746	5.000130653	8.880599022
-0.000000571	3.424746752	11.912997246
4.703761578	6.712502956	0.649799883
1.567920446	5.205614567	1.082999706
3.919801950	5.137119770	3.682199478
-1.567920804	5.068625450	6.281399250
0.783959746	3.630231380	4.115399361
3.135839939	3.561736345	6.714599133
-2.351881504	3.493242264	9.313798904
-0.000000570	2.054847956	7.147799015
2.351880550	1.986353159	9.746998787
-0.783960640	0.479464889	10.180198669
1.567920446	0.410970241	12.779397011
6.271682739	3.698725939	1.516199827
3.135840893	2.191837788	1.949399710
5.487721443	2.123342752	4.548598766
2.351881027	0.616454661	4.981799126
4.703761101	0.547959745	7.580998898
1.567920208	-0.958928585	8.014199257
3.919800758	-1.027423739	10.613398552
-1.567920923	-1.095918298	13.212597847
0.783959508	-2.534312248	11.046598434
3.135840416	-2.602806568	13.645797729
-0.000000095	0.684949458	2.382599592
-0.000000369	8.219390869	0.216599911
2.351880550	8.150896072	2.815799713
-0.783960462	-0.890433908	5.414999485
-0.783960700	6.644008636	3.248999596
1.567920208	6.575513840	5.848199368
3.919800997	6.507018089	8.447399139
-0.783960581	7.328958511	5.631599426
-1.567920804	5.753574371	8.663997650
0.783959806	5.685079098	11.263198853
-2.351881504	4.178191662	11.696398735
2.351880550	7.465947151	0.433199853
4.703761578	7.397451878	3.032399654
-0.783960402	5.959058285	0.866399884
1.567920446	5.890563965	3.465599537
3.919800520	5.822069645	6.064799309
-1.567920804	4.383675575	3.898799419
0.783959925	4.315180779	6.497999191
3.135841131	4.246685505	9.097197533
-2.351881027	2.808292389	6.931199074

-0.000000381	2.739797831	9.530398369
2.351880074	2.671302557	12.129598618
-0.783960998	1.164414048	12.562798500
3.919800997	4.452170372	1.299599886
0.783960223	2.945281982	1.732799768
3.135840893	2.876787186	4.331998825
-0.000000191	1.369898915	4.765199184
2.351879835	1.301403761	7.364398956
4.703762054	1.232909322	9.963598251
-0.783960521	-0.205484524	7.797598839
1.567919970	-0.273979366	10.396799088
3.919800043	-0.342474222	12.995998383
-1.567920923	-1.780867815	10.829998970
0.783959329	-1.849362612	13.429198265
5.487722397	1.438393593	2.165999413
0.000000000	0.000000000	0.000000000
2.351880550	-0.068494841	2.599199772
4.703761101	-0.136989683	5.198399544
3.919800282	-1.712372899	8.230798721

S15

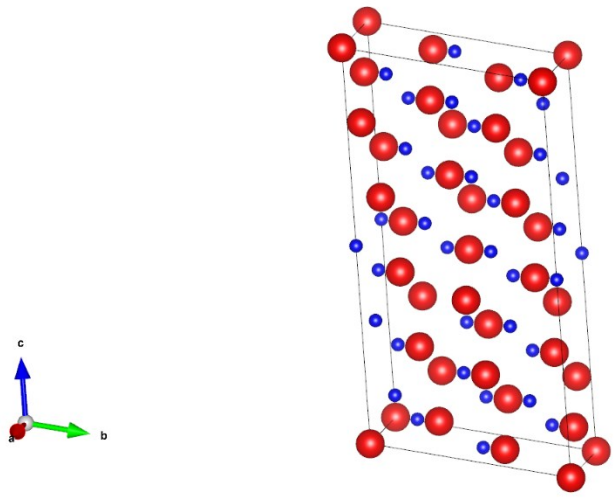

Figure S15. **$PuC_{0.484}(Pu_{32}C_{31})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T15

Table T15. **$PuC_{0.484}(Pu_{32}C_{31})$**

PuC31
1.0
6.0725297928 0.0000000000 0.0000000000
0.0000000000 9.2759428024 0.0000000000
-2.0241764661 -3.9754047511 17.3114873165
C Pu
31 32
Cartesian
4.048353672 1.325134039 15.688535690
4.048353195 2.650269032 12.442631721
4.048353195 3.975403786 9.196727753
4.048353195 5.300538540 5.950823784
-1.012088180 -1.987702370 8.655743599
4.048353672 6.625673294 2.704919815
5.060441494 -0.662567616 5.409839630
5.060441494 0.662567258 2.163935900
3.036264896 4.637971401 0.000000000
1.012088776 1.987701297 14.065583229
2.024177074 3.975403547 16.770503998
1.012088537 3.312836409 10.819679260
2.024176836 5.300538540 13.524599075
3.036265135 -1.987702489 16.229518890
1.012088299 4.637970924 7.573775768
2.024177074 6.625673294 10.278695107
3.036265373 -0.662568092 12.983615875
0.000000052 3.975404024 1.622951984
1.012088299 5.963105679 4.327871799
2.024176598 -1.325134993 7.032791615
3.036265612 0.662567019 9.737711906
2.024176598 -0.000000179 3.786887884
3.036264896 3.312836647 3.245903969
1.012088418 7.288240910 1.081967950
-1.012088060 4.637970924 15.147551537
2.024176598 1.325134754 0.540983975
-1.012088060 5.963105679 11.901647568
0.000000171 -1.325135231 14.606567383
0.000000305 -0.000000536 11.360663414
0.000000022 1.325134277 8.114759445
0.000000156 2.650269270 4.868855953
4.048353195 -2.650269985 14.065583229
4.048354149 -1.325135350 10.819679260
4.048353195 -0.000000358 7.573775768
4.048353672 1.325134516 4.327871799
5.060441971 3.312836409 7.032791615

4.048353195	2.650269508	1.081967950
5.060441494	4.637971401	3.786887884
5.060441494	5.963106155	0.540984035
1.012088418	-3.312837124	15.688535690
1.012088895	-1.987702608	12.442631721
2.024176598	-0.000000715	15.147551537
1.012088418	-0.662567556	9.196727753
2.024176598	1.325134397	11.901647568
3.036265135	3.312835932	14.606567383
1.012088299	0.662567198	5.950823784
2.024176598	2.650269032	8.655743599
3.036265373	4.637970924	11.360663414
0.000000000	0.000000000	0.000000000
1.012088537	1.987701893	2.704919815
2.024177074	3.975403786	5.409839630
3.036264896	5.963105679	8.114759445
2.024176836	5.300539017	2.163935900
3.036265135	7.288240910	4.868855953
3.036265135	8.613375664	1.622951984
-1.012087941	-0.662568271	16.770503998
-1.012088180	0.662566841	13.524599075
0.000000045	2.650268555	16.229518890
-1.012088180	1.987701654	10.278695107
0.000000179	3.975403309	12.983615875
0.000000313	5.300538540	9.737711906
0.000000030	6.625673294	6.491807938
0.000000104	7.950808048	3.245903969

S16

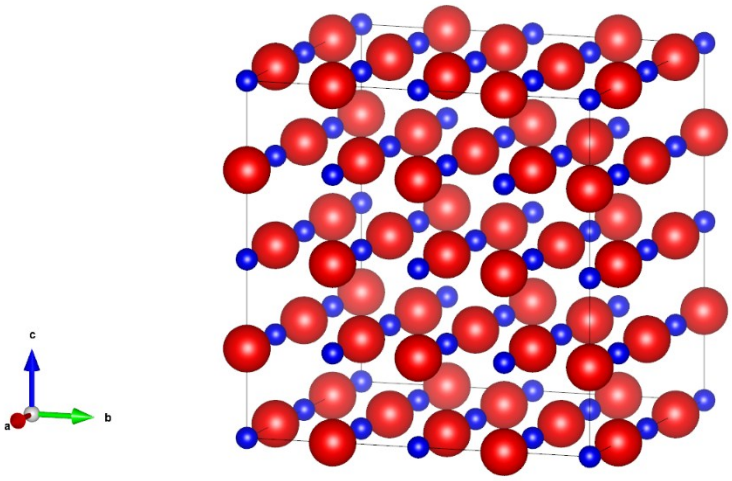

Figure S16. **$PuC_{0.5}(Pu_{32}C_{32})$** Red and Blue ball represent Pu-atom, C-atom respectively.

T16

Table T16. **$PuC_{0.5}(Pu_{32}C_{32})$**

PuC32
1.0

9.9163999557	0.0000000000	0.0000000000
0.0000000000	9.9163999557	0.0000000000
0.0000000000	0.0000000000	9.9163999557

C Pu
32 32
Cartesian

0.000000000	0.000000000	0.000000000
4.958199978	0.000000000	0.000000000
0.000000000	4.958199978	0.000000000
4.958199978	4.958199978	0.000000000
0.000000000	0.000000000	4.958199978
4.958199978	0.000000000	4.958199978
0.000000000	4.958199978	4.958199978
4.958199978	4.958199978	4.958199978
0.000000000	2.479099989	2.479099989
4.958199978	2.479099989	2.479099989
0.000000000	7.437299728	2.479099989
4.958199978	7.437299728	2.479099989
0.000000000	2.479099989	7.437299728
4.958199978	2.479099989	7.437299728
0.000000000	7.437299728	7.437299728
4.958199978	7.437299728	7.437299728
2.479099989	0.000000000	2.479099989
7.437299728	0.000000000	2.479099989
2.479099989	4.958199978	2.479099989
7.437299728	4.958199978	2.479099989
2.479099989	0.000000000	7.437299728
7.437299728	0.000000000	7.437299728
2.479099989	4.958199978	7.437299728
7.437299728	4.958199978	7.437299728
2.479099989	2.479099989	0.000000000
7.437299728	2.479099989	0.000000000
2.479099989	7.437299728	0.000000000
7.437299728	7.437299728	0.000000000
2.479099989	2.479099989	4.958199978

7.437299728	2.479099989	4.958199978
2.479099989	7.437299728	4.958199978
7.437299728	7.437299728	4.958199978
2.479099989	2.479099989	2.479099989
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2.479099989	7.437299728	2.479099989
7.437299728	7.437299728	2.479099989
2.479099989	2.479099989	7.437299728
7.437299728	2.479099989	7.437299728
2.479099989	7.437299728	7.437299728
7.437299728	7.437299728	7.437299728
2.479099989	0.000000000	0.000000000
7.437299728	0.000000000	0.000000000
2.479099989	4.958199978	0.000000000
7.437299728	4.958199978	0.000000000
2.479099989	0.000000000	4.958199978
7.437299728	0.000000000	4.958199978
2.479099989	4.958199978	4.958199978
7.437299728	4.958199978	4.958199978
0.000000000	2.479099989	0.000000000
4.958199978	2.479099989	0.000000000
0.000000000	7.437299728	0.000000000
4.958199978	7.437299728	0.000000000
0.000000000	2.479099989	4.958199978
4.958199978	2.479099989	4.958199978
0.000000000	7.437299728	4.958199978
4.958199978	7.437299728	4.958199978
0.000000000	0.000000000	2.479099989
4.958199978	0.000000000	2.479099989
0.000000000	4.958199978	2.479099989
4.958199978	4.958199978	2.479099989
0.000000000	0.000000000	7.437299728
4.958199978	0.000000000	7.437299728
0.000000000	4.958199978	7.437299728
4.958199978	4.958199978	7.437299728

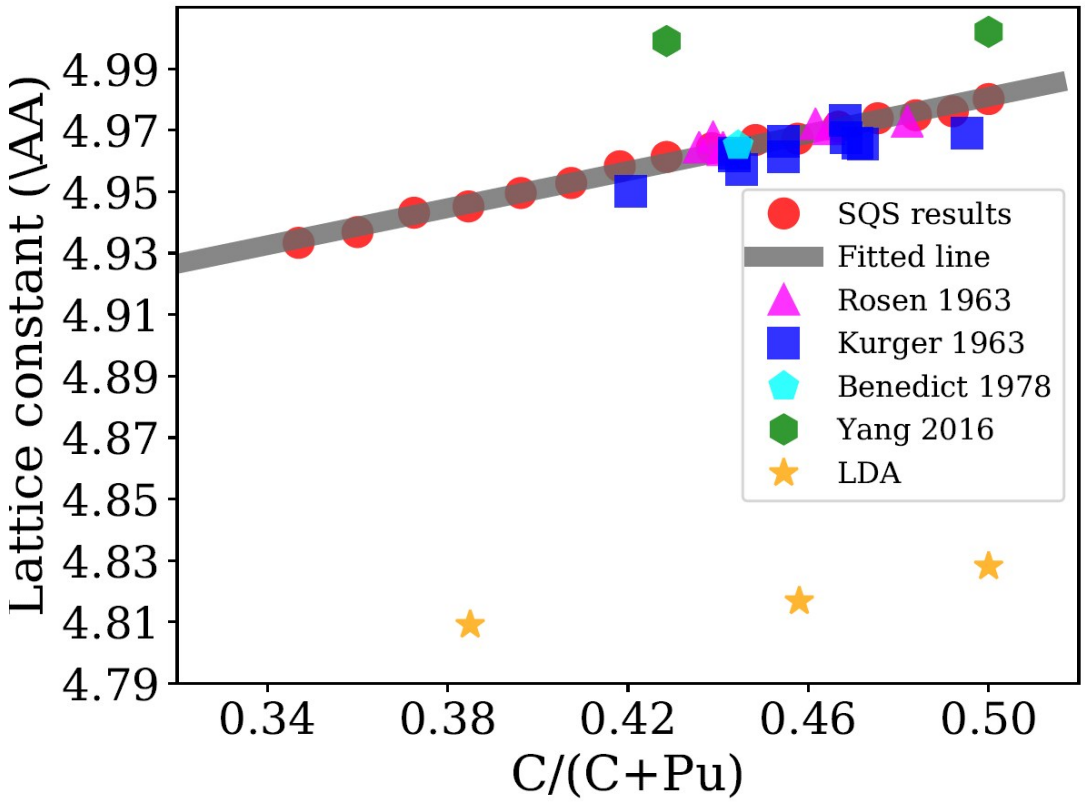

Figure S17. **Lattice comparison with LDA**

One can see that LDA underestimated the lattice parameters of PuC_{1-x} due to its notorious overbinding effect.

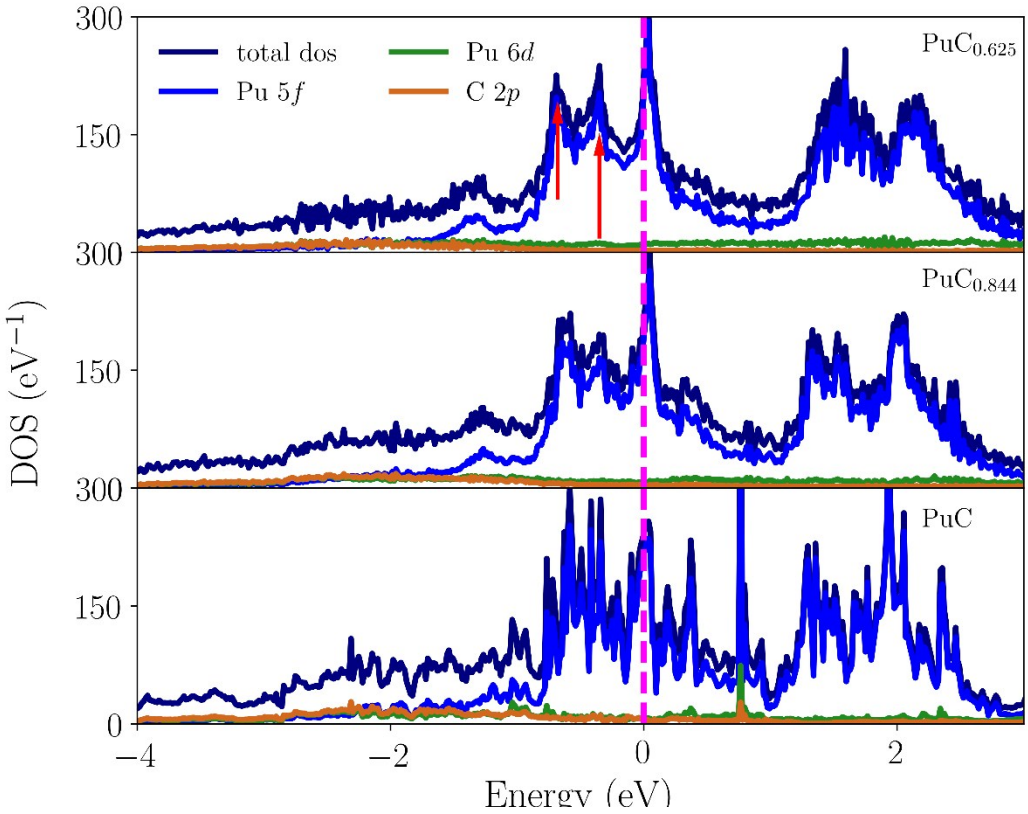

Figure S18. **DOS by LDA**

For the DOS from LDA is very similar to PBE, the microscopic mechanism of stabilization of PuC_{1-x} is likely to be independent of xc functional.

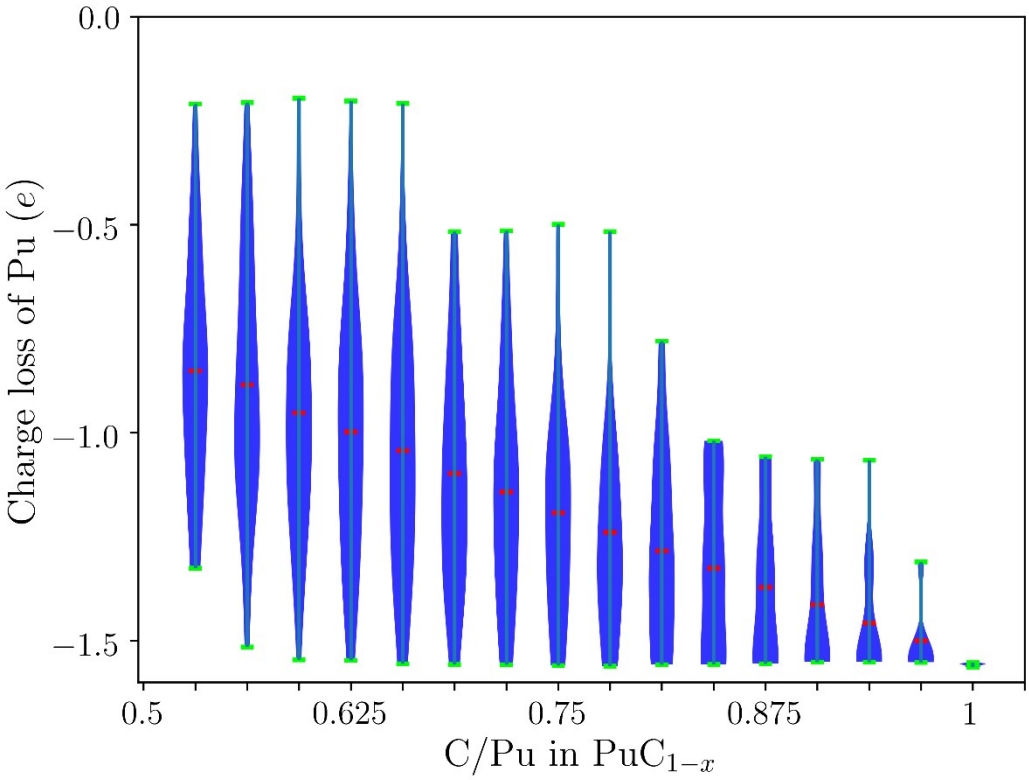

Figure S19. **The violin plot for Bader charge loss of Pu atoms with respect to x. The boundary and mean are represented by green and red bar, respectively.**