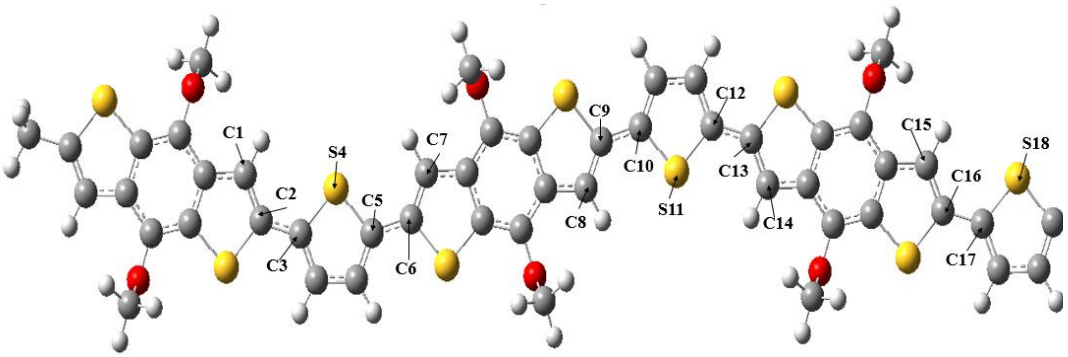
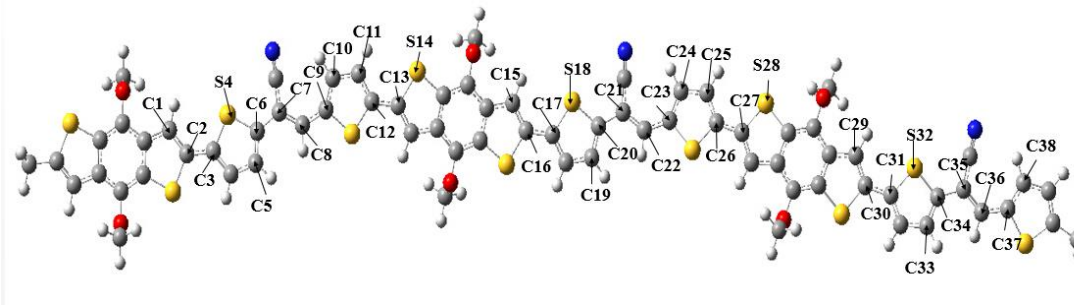
Supporting materials



P1-3



Pb-3

Fig.S1. Labeled graphs of **P1-3** and **Pb-3**

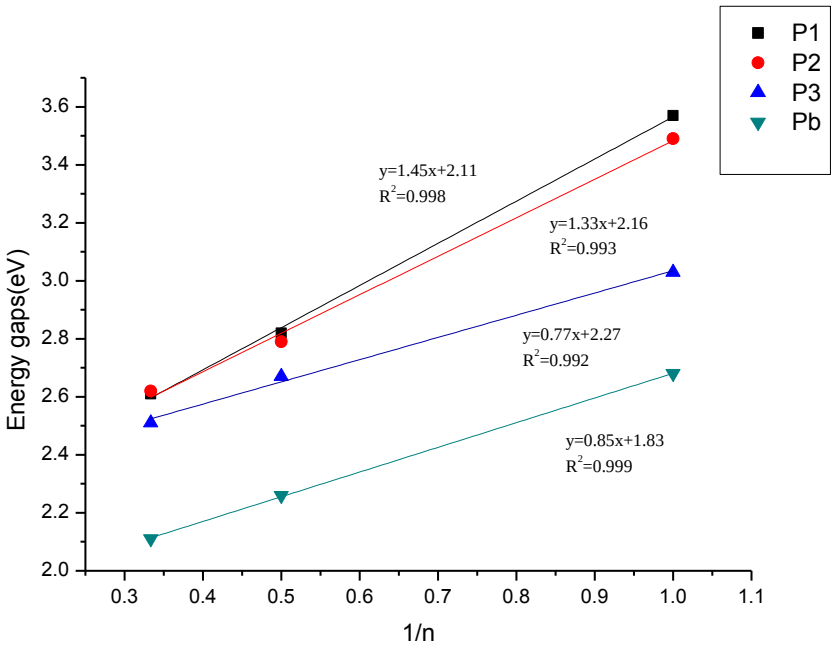


Fig.S2. Relationship between energy gaps and the reciprocal of conjugated unit (1/n).

Table S1 optimized structures (Cartesian x, y, z coordinates) for P1 (N=3).

P1 (Angstroms)		
X	**Y**	**Z**
-14.6587	-0.27799	-0.20564
-14.1365	1.039491	-0.07064
-12.7714	1.301899	-0.0133
-11.8849	0.211365	-0.08326
-12.4079	-1.10598	-0.21729
-13.7729	-1.36723	-0.2741
-16.0967	-0.27947	-0.26186
-16.6532	0.957638	-0.16268
-15.4315	2.226919	0.010881
-10.4542	0.216653	-0.0264
-9.89039	-1.02853	-0.12713
-11.1218	-2.29974	-0.30504
-8.49226	-1.38898	-0.10792
-7.23788	-0.16026	-0.0397
-5.96327	-1.37036	-0.04873
-6.51066	-2.63702	-0.10975
-7.92411	-2.64745	-0.14301
-18.1065	1.320641	-0.18638
-14.2356	-2.65572	-0.43101

-12.3021	2.586693	0.143698
-14.5562	-3.32117	0.7967
-12.0168	3.26694	-1.08551
-2.05199	-1.02781	0.004604
-2.60127	0.279709	0.141877
-1.73524	1.383697	0.25842
-0.36644	1.148962	0.200129
0.182815	-0.15779	0.054934
-0.68304	-1.26529	-0.0275
-3.31504	-2.24074	-0.13505
-4.5719	-0.98986	0.001519
-4.03164	0.263727	0.133573
0.895855	2.36875	0.27191
2.151797	1.121398	0.102586
1.612116	-0.13504	-0.00155
3.541896	1.509333	0.081194
-0.19274	-2.54164	-0.18724
-2.22957	2.663024	0.376253
0.127507	-3.2108	1.039176
-2.47447	3.080282	1.725728
9.46932	-0.04123	-0.07607
9.988411	1.279193	0.052086
11.35167	1.550057	0.070021
12.24295	0.465538	-0.03358

11.7243	-0.85483	-0.16269
10.36092	-1.12588	-0.18018
8.038509	-0.05461	-0.09566
7.470429	1.187174	0.028778
8.698229	2.463959	0.186241
13.67464	0.478896	-0.01258
14.24265	-0.76106	-0.13813
13.01651	-2.03766	-0.29881
15.64663	-1.11384	-0.15486
16.89355	0.121396	-0.24017
18.15203	-1.07178	-0.20787
17.64532	-2.3407	-0.14367
16.2229	-2.36631	-0.11377
9.898723	-2.41366	-0.33284
11.81132	2.838762	0.222992
9.630278	-3.09609	0.899063
12.10168	3.513861	-1.00816
4.083807	2.779652	0.051876
5.49725	2.796963	0.032021
6.070831	1.540369	0.046217
4.821898	0.305408	0.099342
-16.6824	-1.18334	-0.38805
-9.87655	1.124625	0.105343
-5.90786	-3.53878	-0.12417

-8.51246	-3.55767	-0.1867
-18.4142	1.823459	0.738912
-18.7154	0.418508	-0.29987
-18.3423	1.995888	-1.01826
-15.3578	-2.79861	1.333365
-13.6764	-3.3966	1.447386
-12.916	3.353525	-1.70734
-11.2339	2.748094	-1.65244
-4.62829	1.165745	0.209611
2.207571	-1.02936	-0.14629
-0.75896	-3.31177	1.677129
0.910347	-2.67504	1.590349
-1.54998	3.072896	2.315872
-3.21801	2.435383	2.21028
7.462089	-0.96346	-0.22635
14.25111	1.387407	0.119887
19.18791	-0.76198	-0.23963
18.26411	-3.23085	-0.11511
15.64095	-3.27988	-0.05357
8.850366	-2.58219	1.474539
10.53657	-3.17738	1.511277
11.20623	3.591084	-1.63665
12.89176	2.99704	-1.56673
3.476444	3.678197	0.031808

6.081842	3.709926	-0.00444
-14.8931	-4.32292	0.521363
-11.6678	4.263754	-0.80768
0.490525	-4.20188	0.759074
-2.85947	4.100272	1.663681
12.44248	4.514228	-0.73316
9.284334	-4.09475	0.624201
Total energy	-1.612e+05 eV	

Table S2 optimized structures (Cartesian x, y, z coordinates) for P2 (N=3).

P2 (Angstroms)		
X	**Y**	**Z**
16.28287	-0.083	1.45699
15.69832	1.203881	1.62704
14.3409	1.441436	1.43539
13.52835	0.359105	1.050637
14.11355	-0.92748	0.880389
15.47122	-1.1635	1.071105
17.69531	-0.06882	1.732709
18.17614	1.154803	2.081132
16.90946	2.391456	2.092042
12.12359	0.350163	0.770205
11.63759	-0.88095	0.418179
12.90932	-2.12284	0.423315

19.58363	1.527291	2.434195
15.99322	-2.42987	0.920147
13.81464	2.705009	1.58144
16.51124	-2.70127	-0.38783
13.31179	2.988974	2.893627
3.889327	-0.71283	-0.32205
4.514895	0.541123	-0.57857
3.718393	1.690221	-0.74795
2.341	1.553462	-0.62338
1.715291	0.299751	-0.36177
2.508673	-0.8541	-0.22613
5.07488	-1.99383	-0.13998
6.406647	-0.84877	-0.43691
5.939533	0.426924	-0.63321
1.156048	2.845221	-0.74747
-0.16719	1.700105	-0.43682
0.292877	0.422279	-0.25662
-1.53163	2.177232	-0.39936
1.939548	-2.07708	0.047427
4.290174	2.920402	-0.98154
4.498463	3.222766	-2.36725
-1.98735	3.470619	-0.31783
-3.41112	3.607495	-0.27415
-4.04947	2.366149	-0.32564

-2.8823	1.060604	-0.45673
10.28233	-1.24601	0.069078
8.950761	-0.13236	0.318755
7.794164	-1.2621	-0.36572
8.416969	-2.45621	-0.73568
9.824074	-2.4197	-0.47825
7.736782	-3.57423	-1.37345
8.240279	-4.82389	-1.50076
7.612453	-5.94738	-2.15745
6.06012	-5.85432	-2.97759
6.126042	-7.53501	-3.40691
7.269972	-8.13188	-2.95148
8.113622	-7.23132	-2.24397
1.564616	-2.82904	-1.11397
-7.4198	0.755945	-0.01668
-7.94236	1.874398	-0.72716
-9.29476	2.003592	-1.02924
-10.1692	0.99174	-0.59358
-9.64504	-0.1297	0.112508
-8.29222	-0.27	0.395952
-6.00998	0.868963	0.197312
-5.45462	2.011784	-0.32206
-6.67909	3.026832	-1.12404
-11.5912	0.912387	-0.74508

-12.1452	-0.21205	-0.1936
-10.9185	-1.25499	0.559865
-7.82888	-1.35753	1.101762
-9.76799	3.111573	-1.69544
-7.34834	-2.43199	0.284363
-9.83082	2.963878	-3.11958
-17.4419	-0.55599	-0.96434
-13.5373	-0.60581	-0.15578
-14.7512	0.251581	-1.09422
-16.0279	-0.77558	-0.50748
-15.5429	-1.73965	0.362807
-14.1253	-1.62582	0.549785
-16.4024	-2.73016	0.994237
-16.0061	-3.70586	1.842362
-16.8469	-4.69567	2.478115
-18.5869	-4.79092	2.243025
-18.7108	-6.15864	3.306515
-17.4921	-6.52003	3.811336
-16.4351	-5.69063	3.341812
-4.09982	4.881502	-0.12279
-3.54373	6.0961	-0.34021
-4.17674	7.383342	-0.16865
-3.60908	8.615483	-0.42885
-4.47474	9.713258	-0.1684

-5.70175	9.318415	0.291811
-5.82093	7.59181	0.416132
18.31639	-0.95637	1.682853
11.51212	1.244798	0.804657
19.65274	1.931355	3.451802
19.98483	2.288282	1.753322
20.22966	0.646022	2.375413
17.33603	-2.02171	-0.63604
15.72812	-2.61106	-1.15054
14.10582	2.913111	3.646309
12.49472	2.307214	3.160244
6.592592	1.271662	-0.81936
-0.35292	-0.41526	-0.01834
3.549309	3.23282	-2.91679
5.178261	2.498124	-2.83233
-1.31309	4.315097	-0.23035
10.49127	-3.23106	-0.74641
6.749711	-3.36643	-1.77867
9.212345	-5.05607	-1.06803
5.316195	-7.97866	-3.9705
7.503926	-9.17826	-3.1149
9.065329	-7.51231	-1.80449
2.436864	-3.05005	-1.74101
0.817419	-2.28991	-1.7097

-5.43812	0.140076	0.759892
-12.1745	1.691342	-1.22288
-6.50449	-2.10959	-0.3382
-8.1442	-2.82378	-0.36083
-10.5127	2.152369	-3.40299
-8.8377	2.765855	-3.54085
-18.1152	-0.39691	-0.11309
-17.8195	-1.41856	-1.52793
-17.5217	0.320831	-1.61344
-13.5567	-2.27679	1.204861
-17.46	-2.66067	0.745387
-14.9523	-3.79443	2.102601
-19.6762	-6.60982	3.49254
-17.3511	-7.3497	4.495616
-15.3956	-5.81566	3.627578
-5.1374	4.832228	0.197761
-2.51527	6.157592	-0.69339
-2.59418	8.719302	-0.79918
-4.19724	10.75131	-0.316
-6.5455	9.936689	0.567804
12.93691	4.014102	2.860415
16.87923	-3.72928	-0.36276
1.135095	-3.76295	-0.74558
4.948085	4.217451	-2.39725

-7.01788	-3.21335	0.971986
-10.2088	3.912101	-3.50753
Total energy	-2.136e+05 eV	

Table S3 optimized structures (Cartesian x, y, z coordinates) for P3 (N=3).

P3(Angstroms)		
X	**Y**	**Z**
-16.2091	-0.05256	-1.80016
-15.6347	1.23962	-1.96776
-14.2898	1.498162	-1.72412
-13.4813	0.432362	-1.28731
-14.0568	-0.85887	-1.11884
-15.4026	-1.11737	-1.36333
-17.6092	-0.06194	-2.13259
-18.0919	1.148923	-2.52002
-16.842	2.402968	-2.50036
-12.0899	0.445574	-0.9478
-11.6081	-0.77455	-0.5532
-12.8603	-2.03243	-0.59306
-19.4889	1.496614	-2.93448
-15.9145	-2.38595	-1.21779
-13.7701	2.764869	-1.86921
-16.9196	-4.12032	0.085923

-16.4552	-2.67602	0.088865
-13.2449	3.04307	-3.17366
-3.88735	-0.54165	0.335261
-4.51536	0.716641	0.564911
-3.72314	1.870771	0.721185
-2.34388	1.733043	0.612578
-1.71657	0.474314	0.378317
-2.50591	-0.68344	0.254172
-5.07065	-1.82565	0.16447
-6.4042	-0.67627	0.436709
-5.94035	0.603499	0.610393
-1.16173	3.027456	0.72574
0.163222	1.875971	0.456528
-0.29372	0.594869	0.28944
1.530633	2.346558	0.43447
-1.93036	-1.90849	0.00675
-4.3052	3.099719	0.922661
-4.46358	3.467723	2.300405
1.994389	3.638876	0.464828
3.420813	3.761953	0.407229
4.047528	2.510163	0.33638
2.871939	1.216759	0.368104
-10.2654	-1.11497	-0.13403
-8.92069	-0.03123	-0.44399

-7.7919	-1.09258	0.363818
-8.43147	-2.25403	0.820969
-9.83281	-2.24186	0.520165
-7.72703	-3.25765	1.592495
-8.10681	-4.51933	1.956089
-7.29593	-5.40418	2.795127
-5.78989	-4.88561	3.533892
-5.55536	-6.44133	4.266664
-6.57378	-7.30247	3.965723
-7.56522	-6.71428	3.131355
-1.59518	-2.6556	1.183915
7.397331	0.918479	-0.19745
7.932711	1.918474	0.664746
9.28585	1.984916	0.983055
10.14621	1.033589	0.405923
9.609768	0.029794	-0.45268
8.255322	-0.04984	-0.75437
5.989631	1.077165	-0.39319
5.449251	2.143755	0.280566
6.683952	3.019777	1.219568
11.56477	0.907068	0.55389
12.10092	-0.13816	-0.15017
10.86925	-1.02946	-1.06652
7.774424	-1.00837	-1.61439

9.77463	2.97942	1.798858
7.34562	-2.22123	-0.97961
9.811281	2.6413	3.191915
17.44447	-0.33937	0.182142
13.48682	-0.5515	-0.2267
14.77761	0.50611	0.327288
15.99824	-0.65529	-0.07501
15.44171	-1.80918	-0.62271
14.00836	-1.72783	-0.70094
16.29467	-2.9071	-1.02797
15.99254	-4.13113	-1.55432
16.99502	-5.13812	-1.91166
18.71631	-4.87842	-1.68414
19.08976	-6.4492	-2.3231
17.96109	-7.12855	-2.68701
16.76937	-6.38533	-2.45387
4.17122	5.000071	0.327781
3.78988	6.276624	0.631989
4.645925	7.450239	0.451923
4.362916	8.752374	0.809254
5.411033	9.664499	0.504123
6.485388	9.057877	-0.08627
6.236111	7.352719	-0.28361
-9.34631	-5.09893	1.524048

-10.3391	-5.61314	1.199256
2.500216	6.570995	1.189526
1.468321	6.854882	1.647803
14.63966	-4.5392	-1.80144
13.55772	-4.912	-2.01601
-18.2195	-0.95737	-2.09168
-11.4888	1.347763	-0.96843
-19.5229	1.883165	-3.96066
-19.9266	2.262953	-2.28269
-20.1252	0.607677	-2.88645
-17.3461	-4.38036	1.060924
-16.0813	-4.79372	-0.11769
-17.6839	-4.27916	-0.68179
-17.287	-1.98927	0.297378
-15.6805	-2.51049	0.848903
-12.8785	4.071346	-3.14128
-14.0235	2.95547	-3.94099
-12.4177	2.365507	-3.41933
-6.59459	1.451105	0.77808
0.353391	-0.24966	0.080794
-4.9245	4.457328	2.298251
-3.49496	3.516663	2.811716
-5.11604	2.75812	2.824313
1.327376	4.490588	0.490784

-10.5122	-3.02854	0.820194
-6.74637	-2.9486	1.94164
-4.67952	-6.61997	4.875988
-6.6197	-8.32417	4.326127
-8.45077	-7.23476	2.784629
-1.15251	-3.59041	0.834078
-2.48813	-2.87525	1.781574
-0.86943	-2.11277	1.802332
5.410072	0.439284	-1.05045
12.1537	1.580746	1.165968
7.006801	-2.87941	-1.78197
6.51811	-2.03119	-0.28468
8.171453	-2.69857	-0.43896
10.2102	3.517693	3.706725
10.46526	1.778989	3.371795
8.806935	2.419388	3.572396
18.03386	-0.38358	-0.74178
17.88861	-1.04527	0.894867
17.56408	0.664794	0.598334
13.38264	-2.52323	-1.08386
17.35529	-2.71768	-0.88331
20.12104	-6.76906	-2.38841
17.97418	-8.12749	-3.10864
15.77421	-6.7529	-2.67722

5.189085	4.889214	-0.0346
3.428531	9.038939	1.278506
5.365001	10.7271	0.715275
7.411634	9.50514	-0.42141
Total energy	-2.222e+05 eV	

Table S4 optimized structures (Cartesian x, y, z coordinates) for Pb (N=3).

Pb(Angstroms)		
X	**Y**	**Z**
-23.914	2.198524	0.059014
-23.9064	0.790217	-0.15021
-22.7306	0.057101	-0.27312
-21.5083	0.750243	-0.1932
-21.5167	2.159011	0.013948
-22.6932	2.890905	0.135258
-25.2526	2.713821	0.174068
-26.2202	1.766134	0.047757
-25.5441	0.153707	-0.22745
-20.1782	0.233855	-0.31196
-19.2012	1.186711	-0.1854
-19.8843	2.803307	0.100992
-17.7682	1.019566	-0.25274
-17.0396	-0.5735	-0.21902

-15.4216	0.09277	-0.3552
-15.4768	1.473414	-0.41515
-16.7887	1.991382	-0.35212
-14.2538	-0.78242	-0.37865
-27.7054	1.949592	0.117173
-22.6539	4.249715	0.3613
-22.7634	-1.29908	-0.50388
-22.753	5.047746	-0.82461
-22.6894	-2.10515	0.679593
-12.9728	-0.30938	-0.2254
-14.5016	-2.17973	-0.56735
-14.7167	-3.31507	-0.71468
-11.7254	-1.01193	-0.26834
-11.3988	-2.3441	-0.49741
-10.0164	-2.60135	-0.44758
-9.23776	-1.48403	-0.18111
-10.2564	-0.07675	0.012799
-5.63035	-0.56698	0.246831
-5.34387	-1.9375	-0.01974
-4.04787	-2.43827	-0.05503
-2.98623	-1.53714	0.15636
-3.27311	-0.16817	0.4316
-4.57	0.326829	0.494045
-7.03304	-0.2972	0.21077

-7.80313	-1.39974	-0.064
-6.81259	-2.85605	-0.30659
-1.58003	-1.79413	0.125763
-0.80804	-0.68712	0.371252
-1.79911	0.763481	0.645885
0.630929	-0.58704	0.414701
1.646258	-1.99185	0.156423
3.112584	-1.05286	0.375659
2.799321	0.26901	0.637656
1.41246	0.52924	0.655717
4.422833	-1.68609	0.265498
-4.81102	1.659196	0.739145
-3.81247	-3.76226	-0.34216
5.593292	-0.96621	0.232552
4.439386	-3.11548	0.191213
4.437705	-4.2787	0.128651
6.948011	-1.42341	0.160892
7.515362	-2.69245	0.112022
8.920197	-2.67872	0.044628
9.478535	-1.40794	0.041049
8.218083	-0.19961	0.117213
-4.99749	1.982711	2.123629
-3.65864	-4.60362	0.809323
12.85711	0.20987	-0.03202

13.38557	-1.10857	-0.14897
14.74956	-1.36527	-0.22252
15.63068	-0.26719	-0.18692
15.10227	1.051477	-0.06827
13.73862	1.308274	0.00266
11.43056	0.208321	0.050387
10.87242	-1.04404	-0.01504
12.10688	-2.31136	-0.18986
17.05851	-0.26636	-0.27037
17.61731	0.984147	-0.20069
16.38422	2.251935	-0.01959
19.01349	1.348593	-0.24964
20.27014	0.12725	-0.20897
21.53681	1.335532	-0.31787
20.98703	2.602209	-0.38007
19.57522	2.609369	-0.33542
22.94505	0.943734	-0.31607
13.26577	2.592847	0.141758
15.21587	-2.65078	-0.36662
12.94741	3.245546	-1.09531
15.586	-3.29353	0.861616
23.95634	1.840054	-0.07827
23.22961	-0.43596	-0.57079
23.44566	-1.56282	-0.77194

25.37801	1.644246	-0.08472
26.17635	0.543186	-0.35496
27.56111	0.810761	-0.23304
27.85738	2.105522	0.128066
26.39595	3.026948	0.326056
29.20702	2.720814	0.341976
-25.4698	3.759751	0.360684
-19.9695	-0.81031	-0.51635
-14.6003	2.101355	-0.52975
-17.0149	3.050917	-0.40577
-28.1963	1.640524	-0.814
-27.9441	3.00304	0.292299
-28.1488	1.361435	0.930219
-23.7064	4.876092	-1.33969
-21.9275	4.8351	-1.51474
-23.5327	-1.90007	1.350084
-21.7492	-1.93303	1.217859
-12.8908	0.758611	-0.04014
-12.1369	-3.1097	-0.69639
-9.59175	-3.58714	-0.60464
-7.44345	0.694168	0.366572
-1.16741	-2.77232	-0.09412
3.543668	1.033455	0.829862
0.993904	1.511072	0.84998

5.476129	0.114051	0.261081
6.932231	-3.60365	0.126321
9.519893	-3.5817	0.004165
-4.10495	1.735702	2.711072
-5.86299	1.452549	2.539966
-4.56607	-4.59859	1.425278
-2.80456	-4.28666	1.420222
10.84945	1.115036	0.175773
17.63943	-1.17179	-0.40459
21.57932	3.504431	-0.4837
18.98225	3.516232	-0.38934
12.15515	2.709834	-1.6326
13.83143	3.324251	-1.73929
14.72846	-3.3686	1.540964
16.39851	-2.75328	1.362354
23.63444	2.851427	0.157349
25.77922	-0.42454	-0.63225
28.33032	0.065462	-0.4084
29.38588	3.559957	-0.3413
29.98647	1.973001	0.167835
29.32549	3.099701	1.364404
-22.6964	6.088233	-0.49746
-22.7335	-3.14313	0.343466
-5.17382	3.059583	2.162993

-3.48144	-5.61088	0.427338
12.59841	4.245502	-0.8297
15.92585	-4.29456	0.588982
Total energy	-2.211e+05 eV	

Table S5. Transition energy and oscillator strengths for **P1** (N=1,2,3)

Molecule	Units	State	Transition energy(eV/nm)	Strength *f*	Contribution MO
P1	n=1	S1	3.727/332.7	f=0.890	H->L / 0.68423
		S2	4.120/301.0	f=0.177	H-1->L / 0.64369
		S3	4.932/251.4	f=0.115	H->L+2 / 0.47717
		S4	5.146/240.9	f=0.080	H->L+1 /0.49478
		S5	5.306/233.7	f=0.013	H-3->L / 0.47394
		S6	5.354/231.6	f=0.001	H->L+3 / 0.52538
	n=2	S1	3.012/ 411.7	f=2.198	H->L /0.65878
		S2	3.630/ 341.6	f=0.261	H-1->L /0.56681
		S3	3.845/ 322.5	f=0.089	H-2->L /0.56527
		S4	3.957/ 313.4	f=0.061	H-3->L /0.43364
		S5	4.315/ 287.4	f=0.020	H->L+1 /0.38290
		S6	4.483/ 276.6	f=0.159	H->L+2 /0.35387
	n=3	S1	2.815/ 440.5	f=3.552	H->L /0.61449
		S2	3.255/ 380.9	f=0.020	H-1->L /0.45831
		S3	3.595/ 344.9	f=0.464	H-2->L /0.49608
		S4	3.745/ 331.1	f=0.038	H-4->L /0.44023
		S5	3.816/ 324.9	f=0.040	H-3->L /0.36946
		S6	3.973/ 312.1	f=0.265	H-5->L /0.31418

Table S6. Transition energy and oscillator strengths for **P2** (n=1,2,3)

Molecule	Units	State	Transition energy(eV/nm)	Strength *f*	Contribution MO
P2	n=1	S1	3.678/337.1	f=1.230	H->L/0.58747
		S2	4.003/309.8	f=0.609	H->L+1 /0.43904
		S3	4.096/302.7	f=0.141	H-1->L /0.47566
		S4	4.467/277.6	f=0.140	H-2->L /0.43706
		S5	4.765/260.2	f=0.004	H-1->L+1/0.34881
		S6	5.046/245.7	f=0.178	H->L +3/0.43104
	n=2	S1	3.010/ 411.9	f=1.920	H->L /0.64929
		S2	3.612/ 343.3	f=0.758	H-1->L /0.42085
		S3	3.730/ 332.4	f=0.554	H-3->L /0.48493
		S4	3.868/ 320.6	f=0.418	H-2->L /0.29221
		S5	3.948/ 314.1	f=0.113	H-2->L /0.27179
		S6	4.005/ 309.6	f=0.669	H-1->L+2/0.33661
	n=3	S1	2.878/ 430.9	f=2.856	H->L /0.58998
		S2	3.188/ 388.9	f=0.675	H->L+1 /0.46750
		S3	3.601/ 344.4	f=1.096	H-2->L /0.30969
		S4	3.701/ 335.1	f=0.559	H-4->L /0.34570
		S5	3.728/ 332.6	f=0.148	H-5->L /0.46236
		S6	3.824/ 324.2	f=0.118	H->L+4 /0.30523

Table S7. Transition energy and oscillator strengths for **P3** (n=1,2,3)

Molecule	Units	State	Transition energy(eV/nm)	Strength *f*	Contribution MO
P3	n=1	S1	3.617/342.8	f=1.169	H->L /0.41588
		S2	3.722/333.1	f=0.506	H->L+1 /0.57063
		S3	4.063/305.1	f=0.152	H-1->L+1/0.37768
		S4	4.151/298.7	f=0.121	H-1->L+1/0.41171
		S5	4.614/ 268.7	f=0.053	H-1->L /0.42770
		S6	4.794/258.6	f=0.030	H-2->L+1/0.41977
	n=2	S1	2.955/ 419.6	f=1.554	H->L /0.62956
		S2	3.547/349.5	f=1.205	H->L+2 /0.37941
		S3	3.588/ 345.5	f=0.314	H-1->L /0.33957
		S4	3.649/ 339.8	f=0.603	H-1->L+1/0.33821
		S5	3.804/ 325.9	f=0.391	H->L+2 /0.33581
		S6	3.897/ 318.2	f=0.165	H-4->L /0.46412
	n=3	S1	2.210/ 561.0	f=1.264	H->L /0.66110
		S2	2.384/ 520.0	f=0.218	H->L+1 /0.61856
		S3	2.442/ 507.8	f=0.275	H-1->L /0.58972
		S4	2.565/ 483.4	f=0.249	H-1->L+1/0.52039
		S5	2.638/ 469.9	f=0.008	H->L+2 /0.63202
		S6	2.660/ 466.1	f=0.003	H-2->L /0.50962

Table S8. Transition energy and oscillator strengths for**Pb** (n=1,2,3)

Molecule	Units	State	Transition energy(eV/nm)	Strength *f*	Contribution MO
Pb	n=1	S1	3.017/ 411.0	f=1.680	H->L /0.62869
		S2	3.736/ 331.9	f=0.055	H-1->L /0.53791
		S3	4.096/ 302.7	f=0.096	H->L+1 /0.46797
		S4	4.244/ 292.1	f=0.148	H-2->L /0.43668
		S5	4.718/ 262.8	f=0.029	H-1->L+1/0.34503
		S6	4.821/ 257.2	f=0.055	H-3->L /0.31633
	n=2	S1	2.540/ 488.2	f=3.735	H->L /0.61779
		S2	3.033/ 408.8	f=0.247	H->L+1 /0.39538
		S3	3.372/ 367.7	f=0.216	H-1->L /0.41794
		S4	3.579/ 346.5	f=0.070	H-3->L /0.42765
		S5	3.775/ 328.5	f=0.038	H-2->L /0.38127
		S6	3.841/ 322.8	f=0.104	H->L+2 /0.36743
	n=3	S1	2.409/ 514.7	f=6.003	H->L /0.52475
		S2	2.686/ 461.6	f=0.099	H->L+1 /0.47191
		S3	3.030/ 409.2	f=0.583	H-1->L+2/0.29611
		S4	3.283/ 377.7	f=0.030	H-2->L /0.33363
		S5	3.406/ 364.0	f=0.127	H-2->L+1/0.35426
		S6	3.553/ 349.0	f=0.128	H-5->L /0.39837

Table S9. Absorption peaks and oscillator strengths for P1, P2, P3 and Pb (n=1) under an electric field.

Field ($\times 10^{-3}$a.u.)	P1	P2	P3	Pb
1	331.38(0.9388)	339.45(1.1729)	340.49(1.4993)	405.50(1.7719)
2	331.64(0.9755)	345.65(1.0125)	341.51(1.5648)	404.97(1.8280)
3	333.39(0.9984)	356.71(0.7912)	345.32(1.5075)	409.00(1.8501)

Table S10. HOMO, LUMO and band gaps for P1, P2, P3 and Pb (n=1) under an electric field.

	P1			P2			P3			Pb		
Field($\times 10^{-3}$ a.u.)	H	L	Δ_{H-L}	H	L	Δ_{H-L}	H	L	Δ_{H-L}	H	L	Δ_{H-L}
1	-5.04	-1.43	3.61	-4.93	-1.53	3.40	-5.19	-1.91	3.28	-5.06	-2.24	2.82
2	-5.02	-1.40	3.62	-4.78	-1.59	3.19	-5.14	-1.74	3.40	-4.99	-2.11	2.88
3	-4.98	-1.39	3.59	-4.59	-1.66	2.93	-5.00	-1.75	3.25	-4.87	-2.03	2.84