Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Exceptional Metal-Semiconductor-Metal Transition of Lead Apatite via Oxygen Defect Tuning

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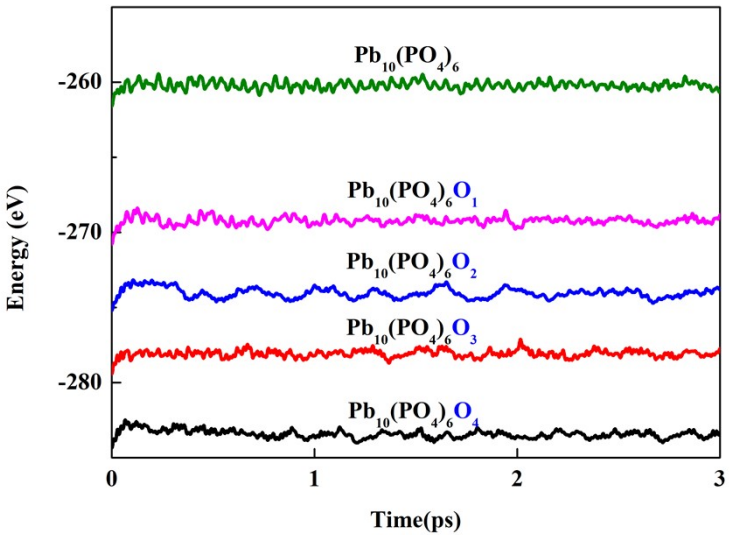

FIG. S1. The AIMD simulations at 300 K for $Pb_{10}(PO_4)O_y$.

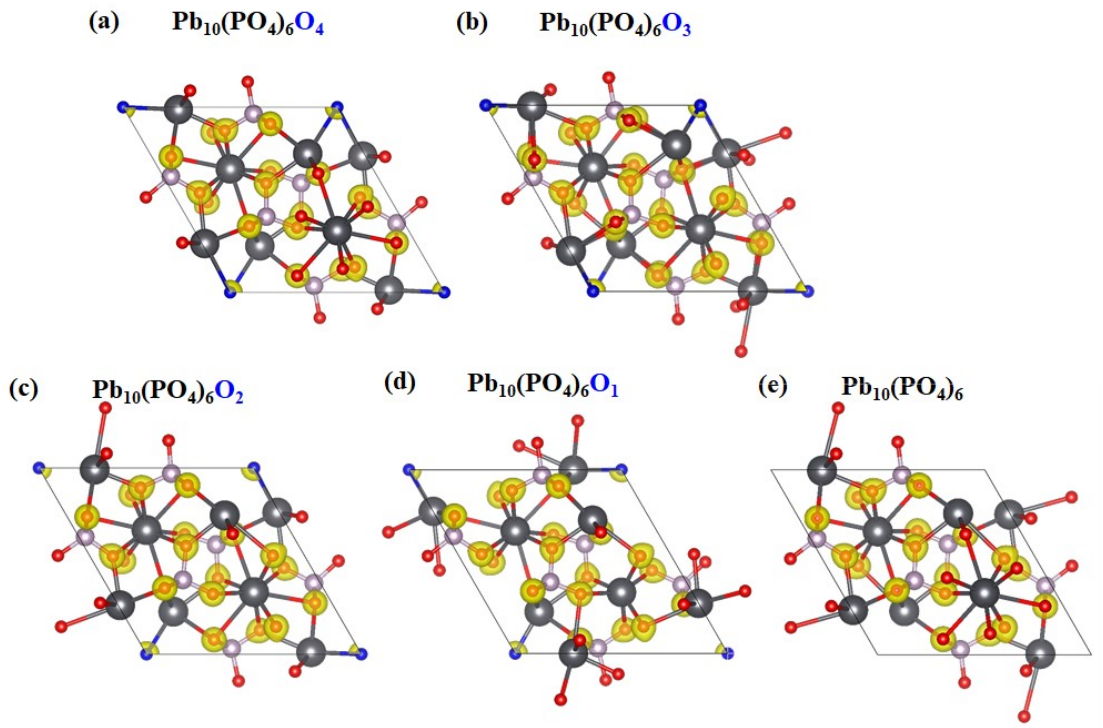

FIG. S2. (a-e) The charge density distribution of $Pb_{10}(PO_x)_6O_y$ structures, where x =4 and y=0-4. The O atoms can be classified into two categories: O (blue sphere) and O (red sphere).

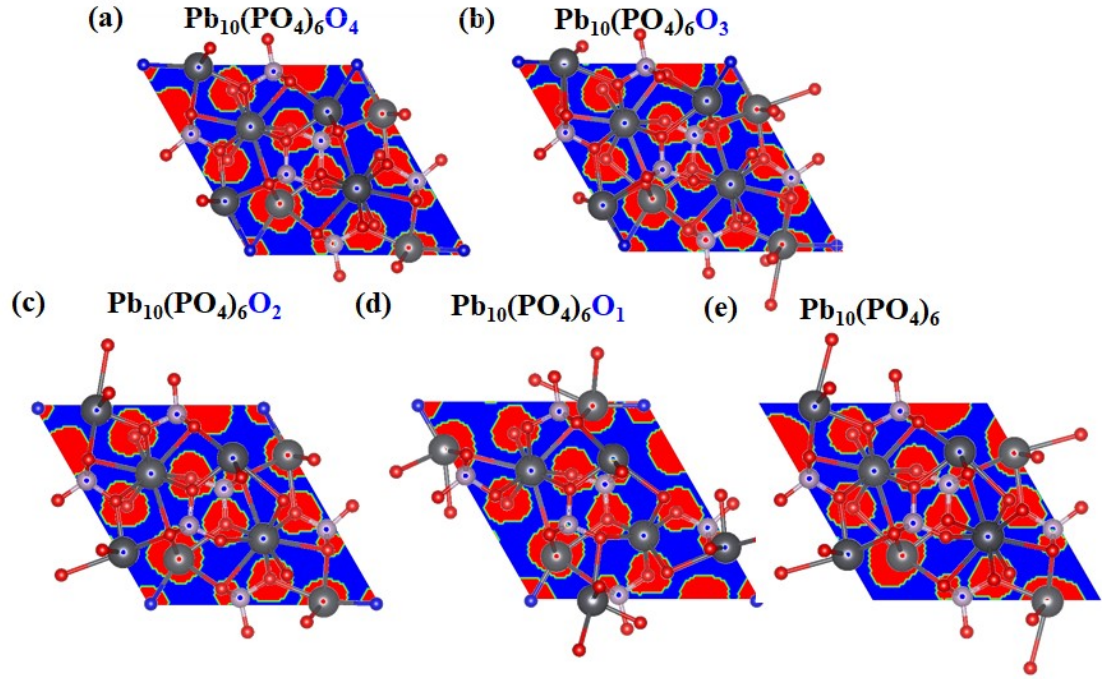

FIG. S3. (a-e) The electron localization function (ELF) of $Pb_{10}(PO_x)_6O_y$ structures, where x =4 and y=0-4.

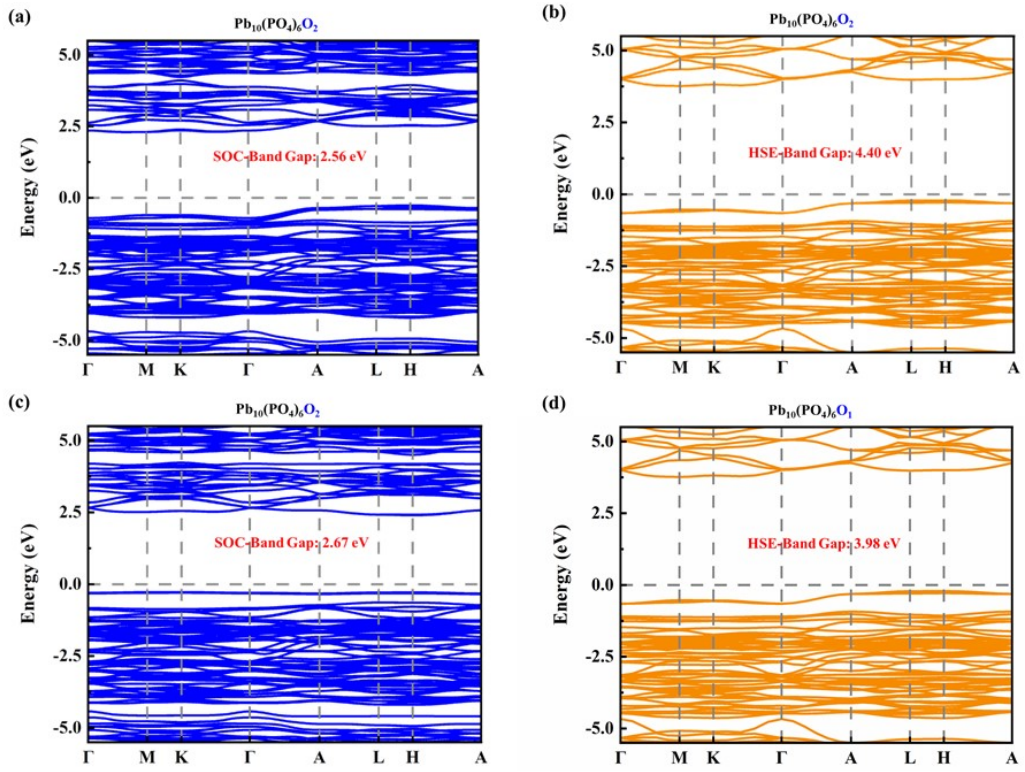

FIG. S4. The band structures of (a-b) $Pb_{10}(PO_4)_6O_2$ and (c-d) $Pb_{10}(PO_4)_6O_2$ using PBE+SOC and HSE functional.

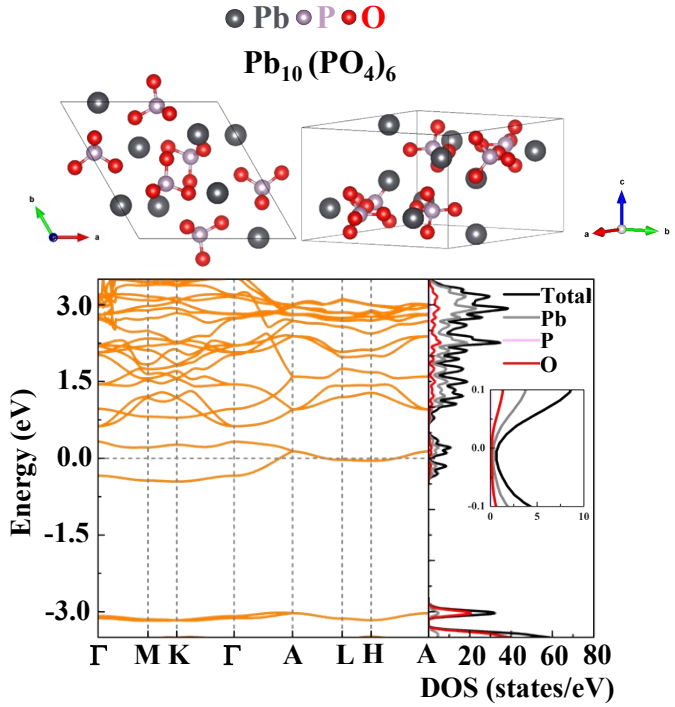

FIG. S5. Optimized top and side views of $Pb_{10}(PO_4)_6$ structures. The corresponding band structures and density of states for these structures are presented below each configurations, respectively. Insets show an amplification of the density of states contributions from various elements near the Fermi level. The lattice parameter of $Pb_{10}(PO_4)_6$ structure are shown in Table 1.

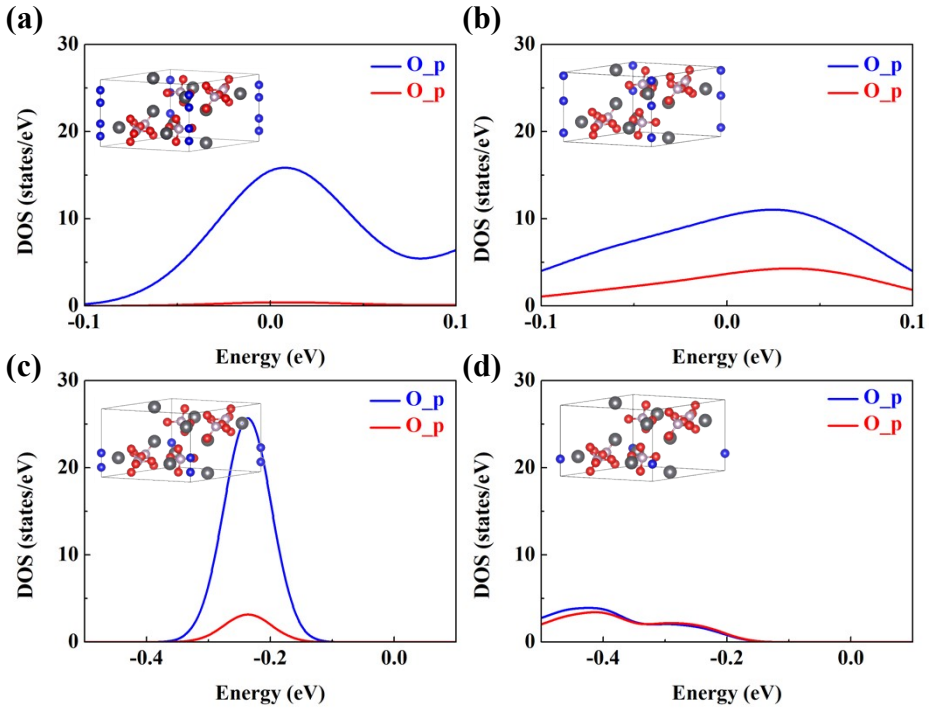

FIG. S6. (a-d) Partial density of states for $Pb_{10}(PO_4)_6O_y$ (y=1-4). The blue and red lines correspond to the p orbitals of the electronic states for isolated oxygen atoms (blue spheres) and oxygen atoms (red spheres) in PO_4 groups, respectively. The position of the Fermi level is marked at 0 eV.

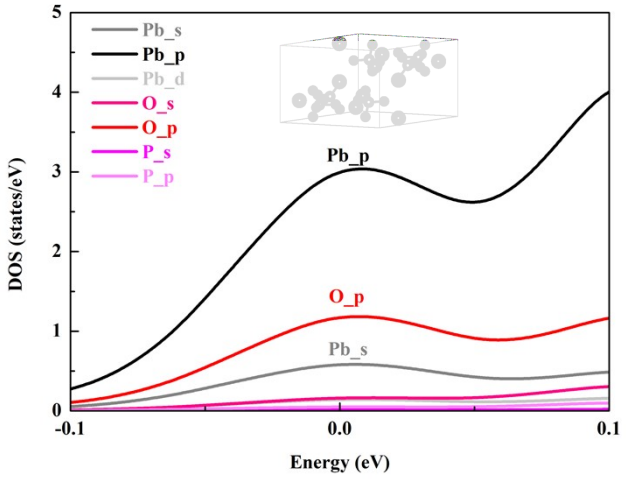

FIG. S7. Partial density of states for $Pb_{10}(PO_4)_6$. The position of the Fermi level is marked at 0 eV.

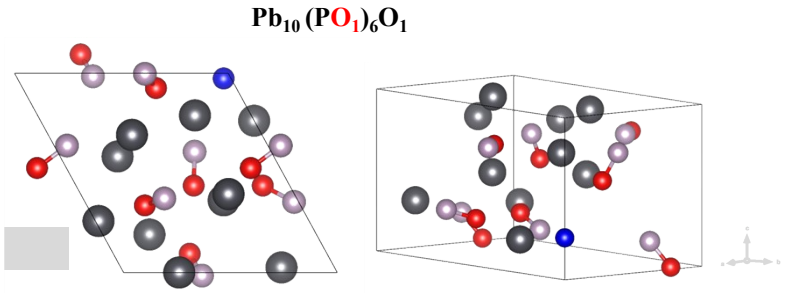

FIG. S8. Top and side views of $Pb_{10}(PO_4)_6\ O_1$ structures after undergoing 1000 optimization steps.

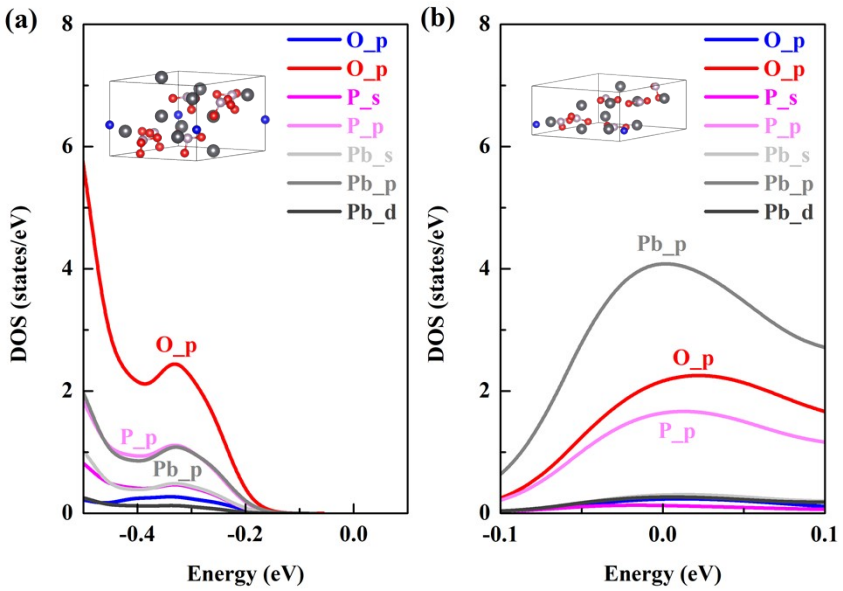

FIG. S9. (a-b) Partial density of states for $Pb_{10}(PO_3)_6O_1$ and $Pb_{10}(PO_2)_6O_1$. The position of the Fermi level is marked at 0 eV.

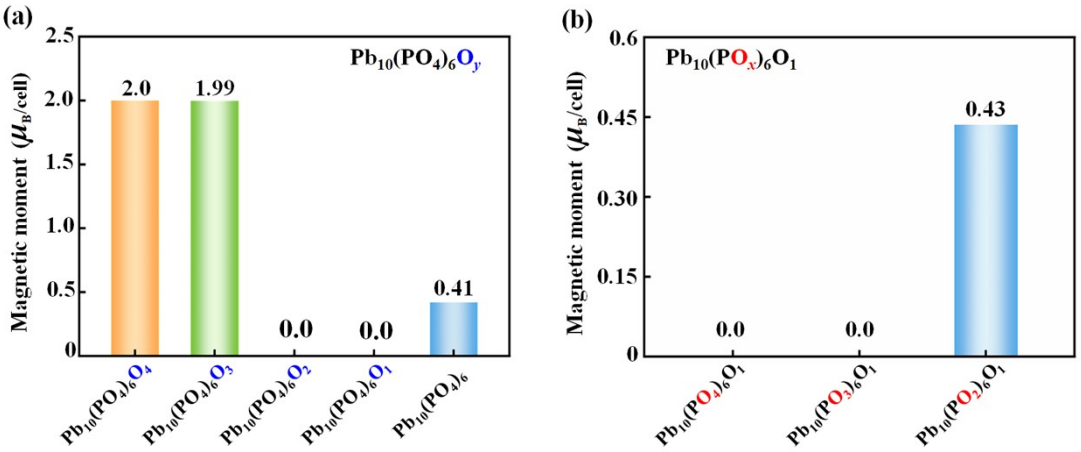

FIG. S10. The magnetic moment of $Pb_{10}(PO_x)_6O_y$ structures with various (a) O_y defects and (b) O_x defects.

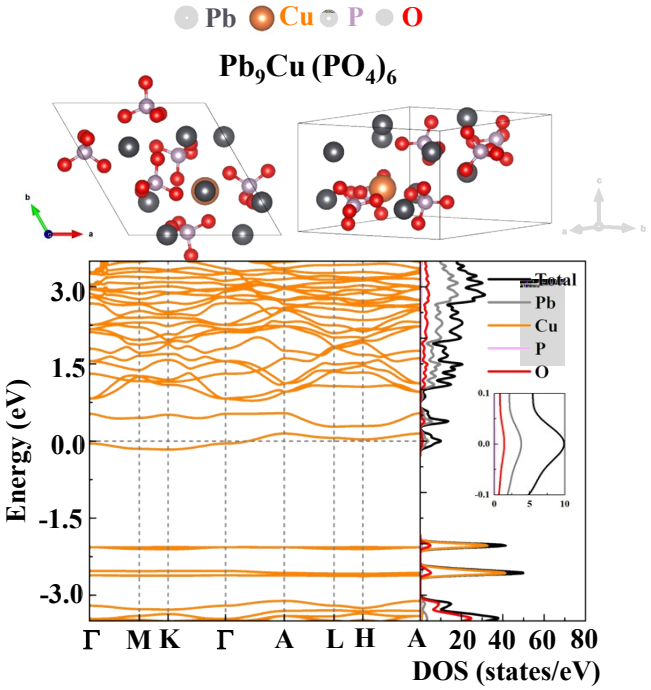

FIG. S11. (a-d) Optimized top and side views of $Pb_9Cu(PO_4)_6$ structures. The Cu atom locate at site 1. The corresponding band structures and density of states for th structures are presented below the configurations. Insets show an amplification of the density of states contributions from various elements near the Fermi level. The lattice parameter of $Pb_9Cu(PO_4)_6$ structure are shown in Table S1.

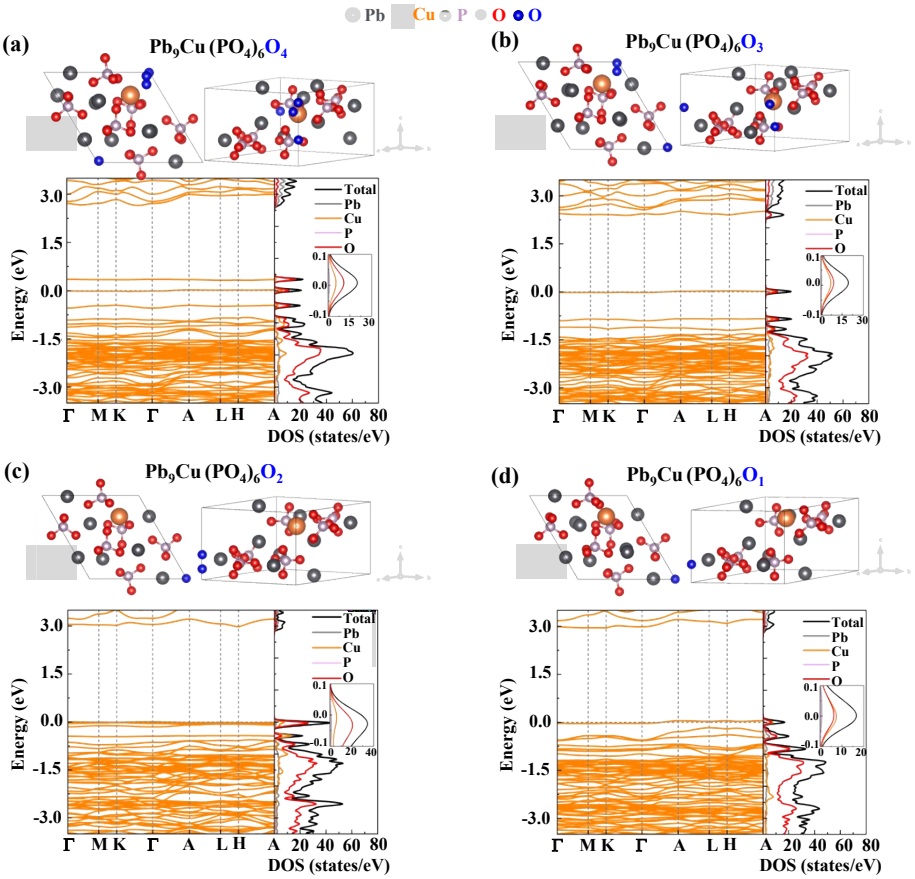

FIG. S12. (a-d) Top and side views of optimized $Pb_9Cu(PO_x)_6O_y$ structures, where x =4 and y=1-4. The Cu atom locate at site 2 and O atoms can be classified into two categories: O (blue sphere) and O (red sphere). The corresponding band structures and DOS for these structures are presented below each configurations. Insets show an amplification of the DOS contribution from various elements near the Fermi level. The lattice parameters of $Pb_9Cu(PO_x)_6O_y$ structures are shown in Table S2.

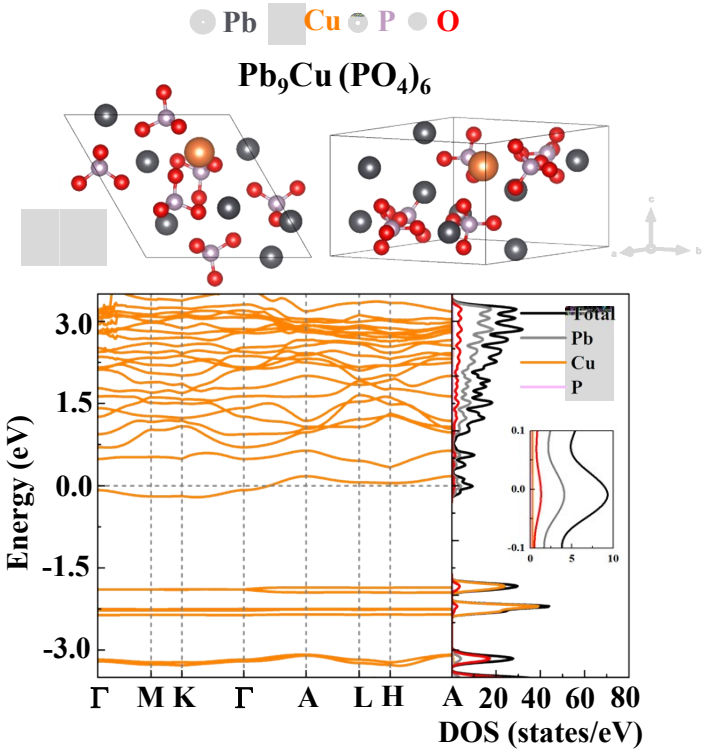

FIG. S13. (a-d) Optimized top and side views of $Pb_9Cu(PO_4)_6$ structures. The Cu atom locate at site 2. The corresponding band structures and density of states for the structure are presented below the configurations. Insets show an amplification of the density of states contributions from various elements near the Fermi level. The lattice parameter of $Pb_9Cu(PO_4)_6$ structure are shown in Table S2.

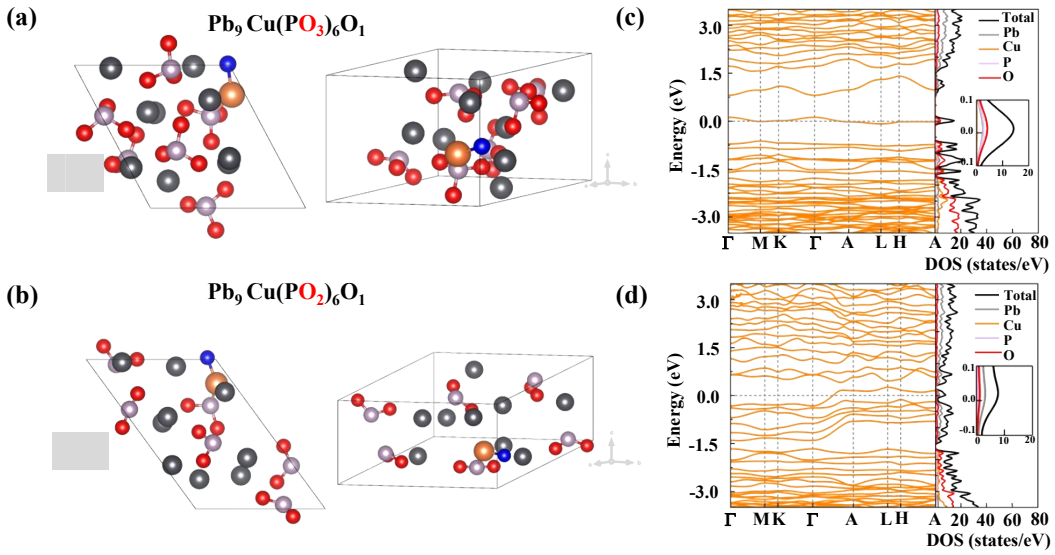

FIG. S14. (a-b) Top and side views of optimized $Pb_9Cu(PO_x)_6O_1$ structures, where x =2,3. The Cu atom locate at site 2 and O atoms can be classified into two categories: O (blue sphere) and

O (red sphere). (c-d) The band structures and DOS for these structures, respectively. Insets show an amplification of the DOS contributions from various elements near the Fermi level. The lattice parameters of $Pb_{10}(PO_x)_6O_y$ structures are shown in Table S4.

Table S1. Independent elastic constants of the $Pb_{10}(PO_4)O_y$, in GPa.

$Pb_{10}(PO_4)O_y$	C_{11}	C_{12}	C_{22}	C_{66}
$Pb_{10}(PO_4)O_4$	82.15	31.84	82.15	23.63
$Pb_{10}(PO_4)O_3$	78.48	18.85	78.55	26.21
$Pb_{10}(PO_4)O_2$	82.14	21.66	82.14	25.85
$Pb_{10}(PO_4)O_1$	82.32	28.46	82.32	14.82
$Pb_{10}(PO_4)$	84.98	24.68	84.98	30.97

Table S2. The DFT relaxed lattice parameters *a*, *b*, *c* (in Å), space group and band gap (in eV) of $Pb_9Cu(PO_4)_6O_4$, $Pb_9Cu(PO_4)_6O_3$, $Pb_9Cu(PO_4)_6O_2$, $Pb_9Cu(PO_4)_6O_1$ and $Pb_9Cu(PO_4)_6$. The Cu atom locate at site 1.

$Pb_9Cu(PO_4)_6O_x$	*a*	*b*	*c*	Space group	Band gap
$Pb_9Cu(PO_4)_6O_4$	10.06	10.29	7.36	P3	Metal
$Pb_9Cu(PO_4)_6O_3$	10.10	10.01	7.37	P1	Metal
$Pb_9Cu(PO_4)_6O_2$	10.07	10.00	7.33	P1	Metal
$Pb_9Cu(PO_4)_6O_1$	10.04	9.99	7.44	$P6_3/m$	Metal
$Pb_9Cu(PO_4)_6$	9.94	9.94	7.29	P1	Metal

Table S3. The DFT relaxed lattice parameters *a*, *b*, *c* (in Å), space group and band gap (in eV) of $Pb_9Cu(PO_4)_6O_4$, $Pb_9Cu(PO_4)_6O_3$, $Pb_9Cu(PO_4)_6O_2$, $Pb_9Cu(PO_4)_6O_1$ and $Pb_9Cu(PO_4)_6$. The Cu atom locate at site 2.

$Pb_9Cu(PO_4)_6O_x$	*a*	*b*	*c*	Space group	Band gap
$Pb_9Cu(PO_4)_6O_4$	10.14	10.05	7.37	Pm	Metal
$Pb_9Cu(PO_4)_6O_3$	9.38	9.82	7.80	P1	Metal
$Pb_9Cu(PO_4)_6O_2$	9.97	9.90	7.31	Pm	Metal
$Pb_9Cu(PO_4)_6O_1$	10.04	9.91	7.41	P1	Metal
$Pb_9Cu(PO_4)_6$	9.92	9.86	7.35	Pm	Metal

Table S4. The DFT relaxed lattice parameters *a*, *b*, *c* (in Å), space group and band gap (in eV) of $Pb_9Cu(PO_3)_6O_1$ and $Pb_9Cu(PO_2)_6O_1$. The Cu atom locate at site 1.

$Pb_9Cu(PO_x)_6O_1$	*a*	*b*	*c*	Space group	Band gap
$Pb_9Cu(PO_3)_6O_1$	9.54	9.42	8.40	P1	Metal
$Pb_9Cu(PO_2)_6O_1$	9.94	12.25	6.42	P1	Metal

Table S5. The DFT relaxed lattice parameters *a*, *b*, *c* (in Å), space group and band gap (in eV) of $Pb_9Cu(PO_3)_6O_1$ and $Pb_9Cu(PO_2)_6O_1$. The Cu atom locate at site 2.

$Pb_9Cu(PO_x)_6O_1$	*a*	*b*	*c*	Space group	Band gap
$Pb_9Cu(PO_3)_6O_1$	9.38	9.82	7.80	P1	Metal
$Pb_9Cu(PO_2)_6O_1$	9.45	12.87	6.55	P1	Metal

Table S6. Comparisons of the model for $Pb_{10}(PO_4)_6O_y$ in our work with those in reference.

Systems	4 defects	3 defects	2 defects	1 defect	0 defect
reference	$Pb_{10}(PO_4)_6O_4$	×	$Pb_{10}(PO_4)_6O_2$	$Pb_{10}(PO_4)_6O_1$	$Pb_{10}(PO_4)_6$
our	$Pb_{10}(PO_4)_6O_4$	$Pb_{10}(PO_4)_6O_3$	$Pb_{10}(PO_4)_6O_2$	$Pb_{10}(PO_4)_6O_1$	$Pb_{10}(PO_4)_6$

Table S7 The atomic coordinates of $Pb_{10}(PO_4)O_4$

$Pb_{10}(PO_4)O_4$		
$Pb_{10}(PO_4)O_4$		
1.00000000000000		
10.1632326335175058	-0.0000064482819559	0.0000000544963192
-5.0816219136161749	8.8016141093778213	-0.0000000004171524
0.0000000414404380	0.0000000310067856	7.3693523112711965
O Pb P		
28 10 6		
Direct		
0.5376538007480768	0.4110880513745584	0.2500000026295618
0.4623533480265030	0.5889167559126710	0.7499999913098213
0.5889119354908460	0.1265654156894023	0.2500000007348450
0.4110830221221238	0.8734364829498245	0.7500000084453610
0.8734346182058432	0.4623462395675920	0.2500000042293076
0.1265635161875970	0.5376467189841787	0.7499999881461548
0.5132020302156795	0.6502482125257474	0.2500000002100007
0.4868112187578105	0.3497591275475325	0.7499999996827491
0.3497512749657218	0.8629535227491661	0.2499999899115729
0.6502406028839707	0.1370522100233491	0.7500000073548406
0.1370465660452530	0.4867978509973986	0.2499999912703912
0.8629481240604330	0.5131882724572324	0.7500000132514375
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0.0000001672857731	0.0000001217216215	0.6571900108167441
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0.3573948447246117	0.0895987749091295	0.0796449898680993
0.6425967608856663	0.9104033158806308	0.9203569832206345
0.9104012558294783	0.2677958722404337	0.0796450793309376
0.0895968295636664	0.7321938835836024	0.9203572841166278
0.2678062037541377	0.3574029864253510	0.5796429850894431
0.7322041847408564	0.6426054974983452	0.4203549778914497
0.6425967701877839	0.9104033311740580	0.5796430070736424
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0.9104012656753903	0.2677958686118619	0.4203549140508109
-0.0127094155663793	0.7362301959280715	0.2500000170174112
0.0127143836087041	0.2637803448845559	0.7499999670813760
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0.7362195576122809	0.7489345276362290	0.7500000100520564
0.7489398070676959	0.0127098044179449	0.2499999970322816

0.2510657961032051	-0.0127146196700920	0.7499999996218492
0.6666666378817454	0.3333332482472973	0.9954136691342247
0.3333332548160765	0.6666667310347529	0.0045873019580646
0.3333332905780607	0.6666667357346328	0.4954126912064121
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0.3733145595365471	0.4090655879844470	0.7499999977783693
0.4090587794017553	0.0357537319521369	0.2499999962453074
0.5909342526760726	0.9642489945672447	0.7500000045019787
0.9642464182549144	0.3733048969318792	0.2499999870969260
0.0357503226053890	0.6266847370272385	0.7500000166901186

Table S8 The atomic coordinates of $Pb_{10}(PO_4)O_3$

$Pb_{10}(PO_4)O_3$		
$Pb_{10}(PO_4)O_3$		
1.0000000000000000		
9.9679046299673413	0.0002568371992084	0.0003054052922623
-4.9837299171906135	8.6333296533916446	-0.0002453755760438
0.0002290998302081	-0.0000762867428765	7.4790584440984418
O Pb P		
27 10 6		
Direct		
0.7399468100324537	0.6419516587455454	0.1005251865958024
0.3580688407554396	0.0980230880804548	0.1005510513473862
0.9019939913501088	0.2600441977815829	0.1005168924783082
0.2668485498222675	0.3366897165711431	0.6099659124923392
0.6632775213678178	0.9301777171459586	0.6099157085335134
0.0697571427181560	0.7331265351574273	0.6100146844426857
0.2921474191401993	0.3730878286006005	0.9464973094567750
0.6269524174825596	0.9191065892645129	0.9464417109278541
0.0808911296478014	0.7077964599162212	0.9465277600534159
0.7410020822484522	0.6568412022441261	0.4334365324686945
0.3431871489723266	0.0842013606473177	0.4334521838372706
0.9157966567407374	0.2589661080930748	0.4334158482850509
0.5291527315618638	0.4208493517084832	0.2776580906668145
0.5286969530867969	0.6775376422604632	0.2597555068583544
0.5791645482670129	0.1082885837550777	0.2776654282529950
0.3224505112304403	0.8511908840506884	0.2597516485544223
0.8916459520826646	0.4708215132423735	0.2776698206554541
0.1487935294517863	0.4712542068678736	0.2597465393453806
0.4702911464977519	0.5931293844459202	0.7427182791884791
0.5013190506432723	0.3527213038283851	0.7665274173519523
0.4068316806130495	0.8771933117978269	0.7427499091507277
0.6472168399091012	0.1486058239795102	0.7665251809504661
0.1228266258204439	0.5296912483730678	0.7427151490386874
0.8513795080637768	0.4986279020949873	0.7665401407515157
0.0004413907848350	0.0001082654986747	-0.0482809441334315
0.0000623063522883	0.0000282975159552	0.5893332412920662
0.0001320290393264	0.0000332105151561	0.1287849624654763
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0.2584214616896998	0.2544398827220151	0.2496295520299066
0.7456167036401823	0.0040359166958960	0.2495322413761257
0.0056961822695688	0.2176520405162903	0.7162846679184597
0.7823534808140008	0.7880613895355075	0.7162826745502714
0.2118866827760486	-0.0057517583537432	0.7162137539025851
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0.3333534781521815	0.6666646152220799	0.5124037019154416
0.3332796174529897	0.6666413727391237	0.0077959712439843
0.6666505573518486	0.3333229075309165	0.5246763623971827
0.6315975773529167	0.6019668696022270	0.2656796669677984
0.3980397597108354	0.0296432942853975	0.2656794607280056
0.9703250706936773	0.3683714800780119	0.2656759925253617
0.3850347745691339	0.4130805878601049	0.7684003149935831
0.5869031278312208	0.9719831312217446	0.7683832814721764
0.0279999170957625	0.6149240205042121	0.7684348014563217

Table S9 The atomic coordinates of $Pb_{10}(PO_4)O_2$

$Pb_{10}(PO_4)O_2$		
$Pb_{10}(PO_4)O_2$		
1.0000000000000000		
10.0386096916974754	-0.0000101477013340	-0.0000000657730019
-5.0193136373398826	8.6936988674944313	0.0000002217860100
-0.0000000424481938	0.0000001644094089	7.3744742306568547
O Pb P		
26 10 6		
Direct		
0.7249764103016706	0.6470484223605053	0.0791293733007390
0.3529504785577042	0.0779249429311346	0.0791303949660964
0.9220742648798416	0.2750255038906902	0.0791300256003746
0.2621249478496412	0.3547896564354711	0.5807951539951418
0.6452105823688414	0.9073356552494130	0.5807951493602058
0.0926641611549054	0.7378744234629688	0.5807951450059413
0.2621249371515503	0.3547896020212690	0.9192048518484093
0.6452105770102018	0.9073356558337011	0.9192048465467186
0.0926641737955906	0.7378743999418300	0.9192048827406045
0.7249763747429916	0.6470483399495505	0.4208706618244988
0.3529504358557904	0.0779249064227282	0.4208696212181118
0.9220742703133522	0.2750254898874895	0.4208699711164542
0.5361471190138295	0.4080558345055337	0.2499999655181389
0.4991148812995709	0.6432474149965788	0.2500000033513015
0.5919435821561937	0.1280906172158580	0.2500000353316519
0.3567540460181821	0.8558673935432968	0.2500000079987866
0.8719093674052074	0.4638533138307396	0.2500000008889920
0.1441326299855273	0.5008872444875295	0.2500000049208527
0.4742443208515549	0.5806002729170874	0.7500000250589608
0.4704779618862977	0.3232003136822383	0.7499999886380256
0.4193996355099481	0.8936437530177794	0.7499999933543461
0.6767998656090666	0.1472778531895900	0.7499999844494177
0.1063558207855092	0.5257556075536218	0.7499999901427881
0.8527216521137712	0.5295217182297721	0.7500000097814219
-0.0000008319976233	0.0000001698752887	0.1450755672396861
-0.0000008665763780	0.0000001508644875	0.3549244267966734
-0.0108046065500724	0.7608435445162574	0.2499999857279352
0.2391573929184613	0.2283523153817785	0.2499999238995239
0.7716460441026014	0.0108041525656819	0.2500000202674060
0.0086322687053449	0.2629891151854094	0.7499999525902188
0.7370107357616357	0.7456435319898574	0.7500000719005587
0.2543561954862872	-0.0086331110010163	0.7499999060646465
0.6666673373183566	0.3333340979567029	0.0010555770180093
0.3333329863807435	0.6666668816131190	0.4919920827832692
0.3333329626155449	0.6666669573829048	0.0080079544838125
0.6666673794586701	0.3333342606897632	0.4989444246473552

0.6189961392864159	0.5885367826043226	0.2499999989660118
0.4114628446787798	0.0304576057908985	0.2500000138111393
0.9695420460532849	0.3810054504962698	0.2500000019380375
0.3694326297407632	0.3993262342812938	0.7500000092776586
0.6006741093182292	0.9701066780623308	0.7499999932529958
0.0298930376822367	0.6305671471882960	0.7500000063770828

Table S10 The atomic coordinates of $Pb_{10}(PO_4)O_1$

$Pb_{10}(PO_4)O_1$		
$Pb_{10}(PO_4)O_1$		
1.00000000000000		
10.0700786950221826	-0.0000042023678023	0.0000001229946036
-5.0350429877804030	8.7209413320273121	0.0000000278614617
0.0000000503006751	0.0000001235533185	7.4131082458126505
Pb P O		
10 6 25		
Direct		
1.0011813404322742	0.7735333864573776	0.2468813113766664
-0.0013531660844832	0.2729993672608842	0.7474709263295538
0.2264668022866196	0.2276479875007036	0.2468808269067766
0.7270005710407329	0.7256473512045157	0.7474711833425722
0.7723523637029023	-0.0011811632962841	0.2468809010853514
0.2743526727675784	1.0013529679749436	0.7474712206580582
0.6666665270529833	0.3333333013961371	0.0058555227086033
0.3333330832072720	0.6666665020100664	0.0071701061757470
0.3333338054503294	0.6666666968970630	0.4876727266217928
0.6666666048969486	0.3333330156625853	0.4918458711790679
0.6261039160663564	0.5965308531692133	0.2480666669588271
0.3594292124595316	0.3891589913712749	0.7478080366168091
0.4034692006868761	0.0295729129122589	0.2480666477231315
0.6108409734813026	0.9702702747774382	0.7478080958179306
0.9704271006191504	0.3738961549161092	0.2480665893706787
0.0297295934395709	0.6405705194181269	0.7478082024918649
0.5023796026195668	0.6459513179851305	0.2474987760619894
0.4692380639271800	0.3231323725146252	0.7482974099327397
0.3540484436725539	0.8564280456430468	0.2474987525865240
0.6768676937846494	0.1461056110049281	0.7482973880528203
0.1435718907602743	0.4976204457948324	0.2474988089664377
0.8538943751590451	0.5307618692473771	0.7482975645915731
0.7327383989115014	0.6594860607296016	0.0786506517291561
0.2522911326128597	0.3404738316737433	0.9164239217874731
0.3405140833629775	0.0732523257857783	0.0786507212179371
0.6595261729559332	0.9118172314647476	0.9164239114872246
0.9267478281685002	0.2672615715948480	0.0786506127401277
0.0881829269798597	0.7477086863597564	0.9164242363366010
0.2511749869820299	0.3384484661592507	0.5802119766205541
0.7332116670733865	0.6611054756229422	0.4168629424146322
0.6615514386926599	0.9127264022662245	0.5802118858230578
0.3388948144610867	0.0721062050451762	0.4168630704726724
0.0872734304491643	0.7488252304722821	0.5802122209420109
0.9278938059043046	0.2667883092796414	0.4168629255228800
0.5473026770545176	0.4170121005356930	0.2491308838713073
0.4592684150892850	0.5712308047413625	0.7464322465419021
0.5829879257857562	0.1302904482012452	0.2491307762836777
0.4287691427310589	0.8880373797123693	0.7464323537930370
0.8697095050080250	0.4526971825368758	0.2491307629673749

0.1119624327939822	0.5407316175074578	0.7464320541587580
0.0000001175539137	-0.0000000105113407	0.2429413737340713

Table S11 The atomic coordinates of $Pb_{10}(PO_4)$

$Pb_{10}(PO_4)$		
$Pb_{10}(PO_4)$		
1.00000000000000		
9.9381780979117149	-0.0000077840445691	0.0000000043035612
-4.9690957910867191	8.6067060248142546	-0.0000000148535454
0.0000000072142699	-0.0000000070985151	7.3627069250793991
O Pb P		
24 10 6		
Direct		
0.5321163069521074	0.4163980999561624	0.2499999943951285
0.4678777671369406	0.5836005241415161	0.7499999915166747
0.5836040356735793	0.1157187670912882	0.2500000064641707
0.4163972321386151	0.8842766413162193	0.7499999877056726
0.8842814090678804	0.4678851301708971	0.2499999945142725
0.1157232198793351	0.5321207230309309	0.7499999909206870
0.5191349936160125	0.6680208681307578	0.2500000034173832
0.4808672811759781	0.3319825838357363	0.7499999924307567
0.3319789706788125	0.8511123604849189	0.2499999945298750
0.6680176521832150	0.1488865750425911	0.7500000004802568
0.1488880860969758	0.4808667565190496	0.2499999908797752
0.8511129721792963	0.5191309209234646	0.7500000031018641
0.7371239805556327	0.6516861246524447	0.0797876021617922
0.2628753658227422	0.3483106825927844	0.9202130741146838
0.3483137726862371	0.0854372442382719	0.0797862109001162
0.6516894951094143	0.9145652646785186	0.9202146122159752
0.9145629076048687	0.2628769097774766	0.0797863688268021
0.0854346244358351	0.7371238728183658	0.9202144845601629
0.2628753591926210	0.3483106816599425	0.5797869223046057
0.7371239594562117	0.6516860989885884	0.4202124165503737
0.6516895139342667	0.9145652703056991	0.5797853931963022
0.3483137666427655	0.0854372289262822	0.4202138044645812
0.0854346254464284	0.7371238911475185	0.5797855291802653
0.9145629104788703	0.2628769226778659	0.4202136371726862
-0.0058931813035805	0.7576124742939822	0.2500000024258642
0.0058914836975082	0.2423765027120451	0.7499999899389492
0.2423872106275766	0.2364939221766372	0.2500000296402647
0.7576238509368268	0.7635154256720482	0.7499999724005313
0.7635051628583285	0.0058925981591443	0.2500000040343938
0.2364855127073018	-0.0058908770964822	0.7499999952925802
0.6666665415857006	0.3333336932638853	0.9972650026589450
0.3333334730441992	0.6666663237500475	0.0027294084119015
0.3333334465838164	0.6666663061995495	0.4972705666536753
0.6666665848230121	0.3333337301124368	0.5027350132390715
0.6281572160652075	0.5986275511093133	0.2500000036317371
0.3718418524564627	0.4013722375322312	0.7499999935591324
0.4013728631026168	0.0295274193493360	0.2500000012513802
0.5986273961441650	0.9704719413456400	0.7499999980764822
0.9704717982703724	0.3718447591048072	0.2499999903844418
0.0295288812558670	0.6281561502081102	0.7500000053957957

Table S12 The atomic coordinates of $Pb_{10}(PO_3)O_1$.

$Pb_{10}(PO_3)O_1$		
$Pb_{10}(PO_3)O_1$		
1.00000000000000		
9.6931230972691083	0.0000692507290825	0.0000484312672035
-4.8465016420861486	8.3943926170055700	-0.0000500910756204
0.0000397646976157	-0.0000252675802573	8.0008840558310172
Pb P O		
10 6 19		
Direct		
0.9910665096471610	0.7752210194121623	0.3034935364476817
0.0066725486082897	0.2555162145076822	0.7803627430863178
0.2247795785921813	0.2158467046977616	0.3034969582283717
0.7444762642923036	0.7511559225670130	0.7803692456738954
0.7841547646827910	0.0089301981661304	0.3034941534640868
0.2488411552886927	0.9933287797141537	0.7803836724579659
0.6666675686185797	0.3333339138950077	0.0275043127848119
0.3333321513428426	0.6666654766848604	0.0236835024625213
0.3333276616627351	0.6666687748015614	0.4839697375755836
0.6666629812820756	0.3333332106279551	0.5102098922523856
0.6420622471634871	0.6133915672020654	0.2287369305455716
0.3571524182285472	0.3877986254094751	0.7255626025507310
0.3866182453165599	0.0286761608694943	0.2287478098370169
0.6121941865392274	0.9693588248208171	0.7255586879396266
0.9713327337751991	0.3579400972128933	0.2287353514379372
0.0306368696303110	0.6428424682414040	0.7255565333887608
0.5153884543911753	0.6721353514489234	0.2295578224366178
0.4556337589397627	0.2971697359723119	0.7169453014926599
0.3278693042436275	0.8432518166406658	0.2295728197455832
0.7028303314613851	0.1584688457845886	0.7169410858016644
0.1567430595295946	0.4846075631611328	0.2295634464992059
0.8415328071184249	0.5443676483928276	0.7169421275890673
0.7083041349827299	0.6322379643030038	0.0417463546595687
0.3677623712237675	0.0760598359863293	0.0417590519023715
0.9239416044131444	0.2917019554490854	0.0417440179954229
0.2758857282909771	0.3694321931353126	0.5460356625312497
0.6305692856369471	0.9064492526846093	0.5460395542156847
0.0935473678625093	0.7241233736047914	0.5460372354553393
0.5503478647468184	0.4261587044658429	0.2573546675276860
0.4797231271081444	0.5760757851290432	0.7357349913963311
0.5738489954337934	0.1241883258893302	0.2573588251746320
0.4239170868251872	0.9036589159595212	0.7357111314987508
0.8758123748803436	0.4496540654132241	0.2573559344107619
0.0963453321756043	0.5202692907946989	0.7357157936734107
-0.0000008239349047	0.0000013409543490	0.4161481718607722

Table S13 The atomic coordinates of $Pb_{10}(PO_2)O_1$.

$Pb_{10}(PO_2)O_1$		
$Pb_{10}(PO_2)O_1$		
1.00000000000000		
10.5507274032445437	-0.9214218856769248	-0.2395466777477675
-6.0774121610976364	10.2637955269156382	-0.1621551361626862
-0.2165961455567244	-0.1538217001495218	6.3498447087076313
Pb P O		
10 6 13		

Direct			
	0.9096133706874568	0.8058707812454312	0.2019278045937939
	0.0824566615371072	0.3125089612686123	0.8034218894125267
	0.2063317463779799	0.2356878867843429	0.2126267517324748
	0.7468404435422159	0.6994352705530811	0.6755096332301759
	0.7161076758405041	-0.0101758214844867	0.2000650329873760
	0.3304563564587790	1.0008012200403484	0.7093028494670326
	0.6656750860444741	0.3137242038614260	0.0795781491550077
	0.2404524380263177	0.6207631525148729	0.0895225328679266
	0.2581264689459489	0.6390838669428981	0.5821218250953120
	0.6845550607947873	0.3272257726447917	0.5688826331661679
	0.5923897308829267	0.6273689735444542	0.1416160164910528
	0.3601680327841320	0.3567968512756610	0.6343922703303145
	0.3528587171193520	0.0202579267543214	0.1781900106540791
	0.6539152904436144	0.9697280269948065	0.7139020149247639
	1.0063563487616782	0.3339305515515623	0.3173824187731238
	0.0388466960894430	0.6814410946505252	0.8355907897600032
	0.5125297793263150	0.7022866030624673	0.1284059968022846
	0.8798150549167226	0.5417356255223915	0.7797001963814919
	0.3661082915630804	0.1598485816021825	0.1332022951665537
	0.8571674232051295	0.2375676538654077	0.1581768357199863
	0.3289360400296504	0.4706109102094121	0.6116941217131242
	0.6549045219773971	0.8409875776192970	0.6637636374474483
	0.1039514701660038	0.7638468610991829	0.6310735549710810
	0.4889055159745601	0.4713534768694252	0.1285756556833117
	0.5421058312605619	0.4345380068203126	0.6485755273576229
	0.5314611401267327	0.0737711276366300	0.1888676910522868
	0.4765326227972261	0.9166535818166626	0.6851174110769744
	0.9829007426443949	0.4365015017097469	0.4352641707091754
	-0.0528685003245187	0.0101998030242202	0.2032600822775953