

Intercalation of Ferrocene into Vanadyl Phosphate by Density Functional Theory

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Ferrocene intercalated on the vanadyl phosphate.

Table S1. The different configurations of ferrocene intercalation into the VOPO₄ layer.

The same color represents the identical configuration.

V/VO	0°	45°	90°
E _⊥ -VO	Red	Green	Red
E _⊥ -V	Cyan	Blue	Cyan
S _⊥ -V	Yellow	Orange	Yellow
E _∥ -V	Orange	Light Green	Orange
S _∥ -V	Blue	Blue	Blue
P/P	0°	45°	90°
E _⊥ -P _{VO}	Yellow	Dark Blue	Purple
E _⊥ -P _V	Purple	Dark Blue	Yellow
S _⊥ -P	Red	White	Red
E _∥ -P	Purple	Light Blue	Purple
S _∥ -P	Grey	Grey	Grey

The 17 possibilities of ferrocene intercalated on the vanadyl phosphate.

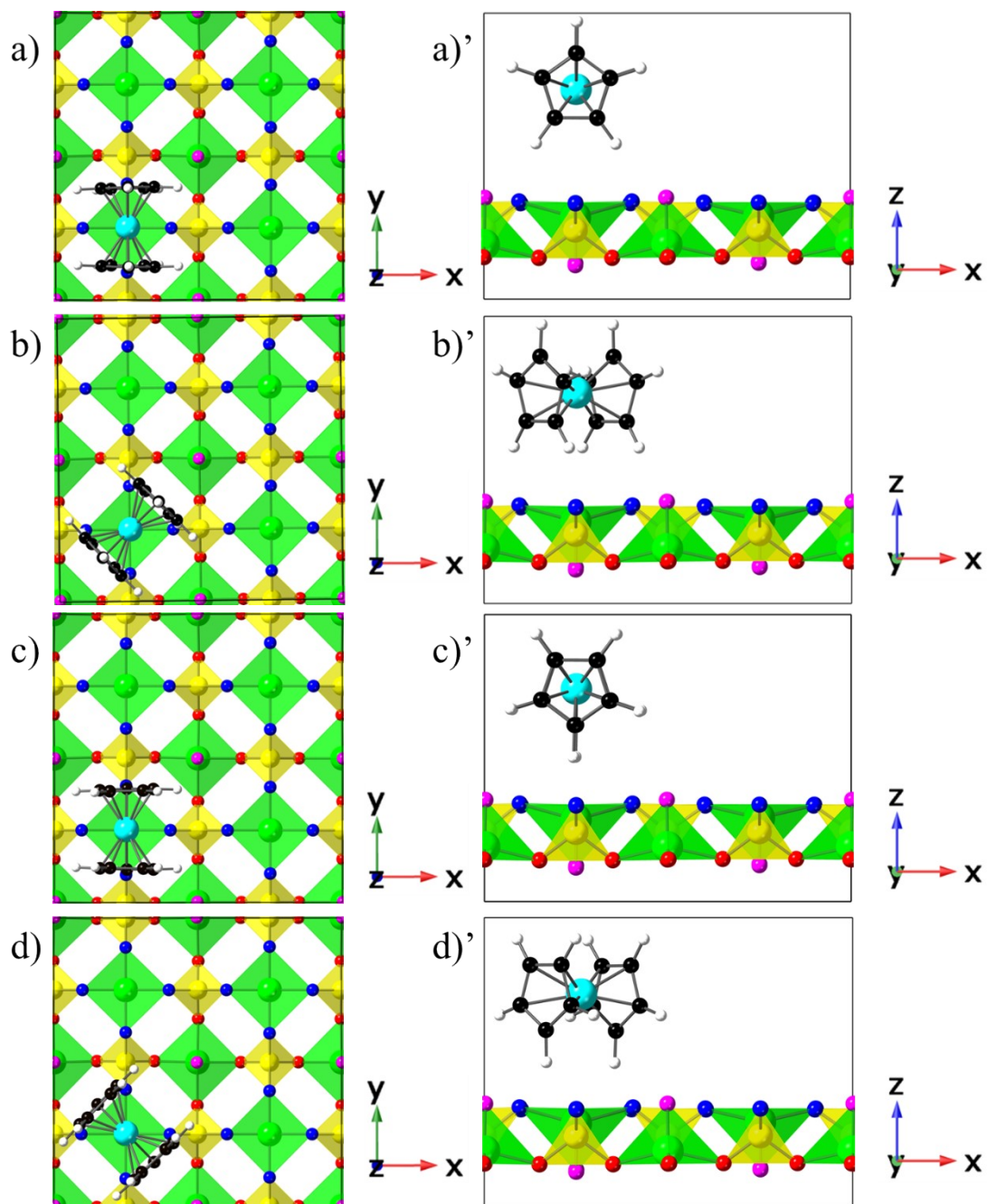


Figure S1. The configurations of a) E_{\perp} -VO- 0° , b) E_{\perp} -VO- 45° , E_{\perp} -V- 0° and d) E_{\perp} -V- 45° are viewed along the [001] direction. The corresponding pictures denoted with prime (') are viewed along the [010] direction. All subsequent configurations are shown in the same directions as these ones. The black box is the unit cell.

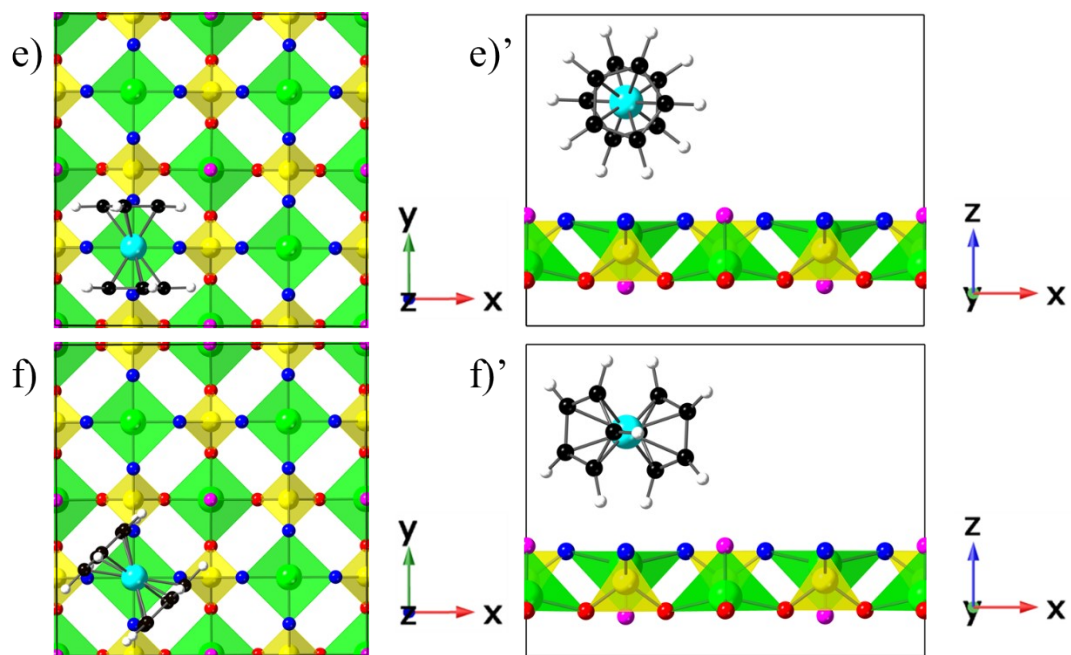


Figure S1. The configurations of e) $S_{\perp}\text{-V-}0^{\circ}$ and f) $S_{\perp}\text{-V-}45^{\circ}$ are viewed along the $[001]$ direction. The corresponding pictures denoted with prime (') are viewed along the $[010]$ direction. The black box is the unit cell.

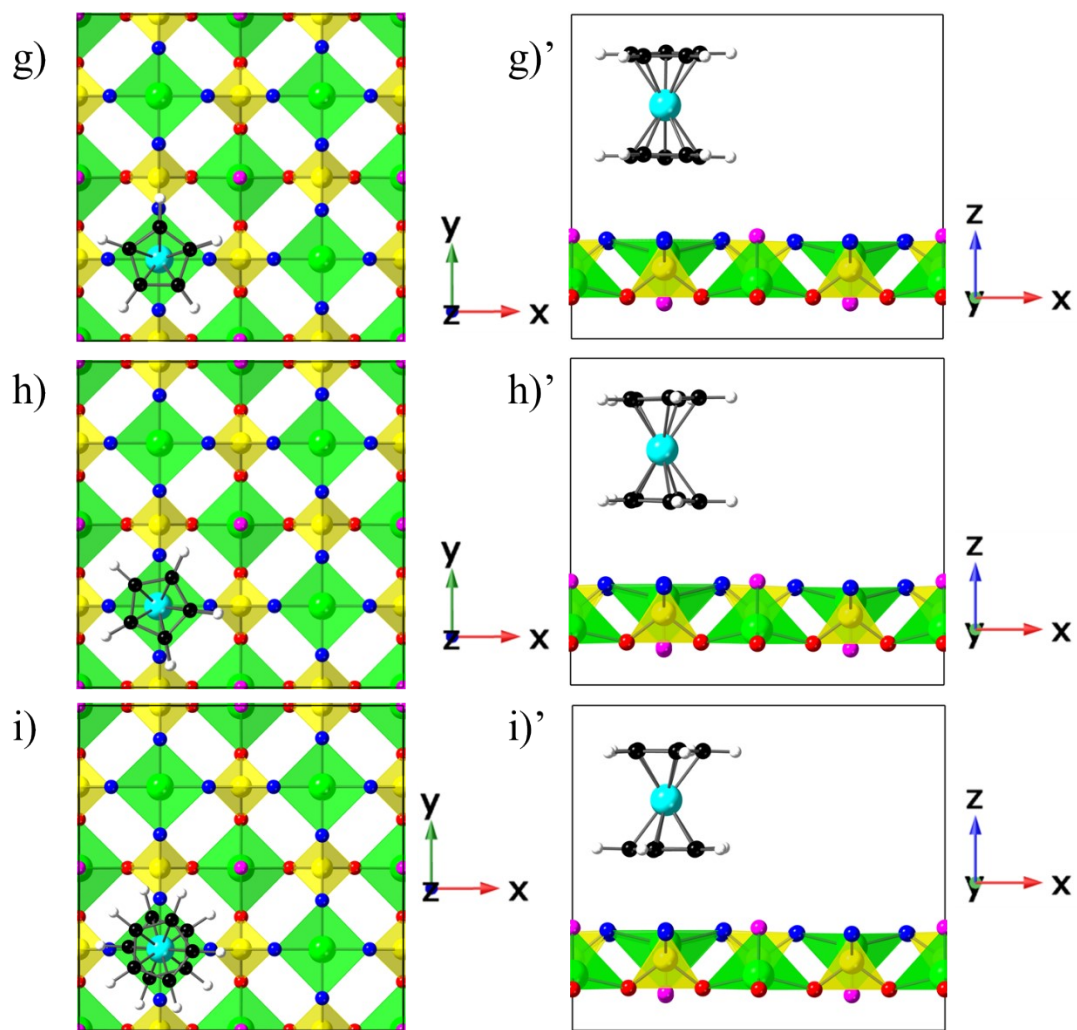


Figure S1. The configurations of g) $E_{\parallel}\text{-V-}0^{\circ}$, h) $E_{\parallel}\text{-V-}45^{\circ}$, and i) $S_{\parallel}\text{-V-}0^{\circ}$ are viewed along the $[001]$ direction. The corresponding pictures denoted with prime ($'$) are viewed along the $[010]$ direction. The black box is the unit cell.

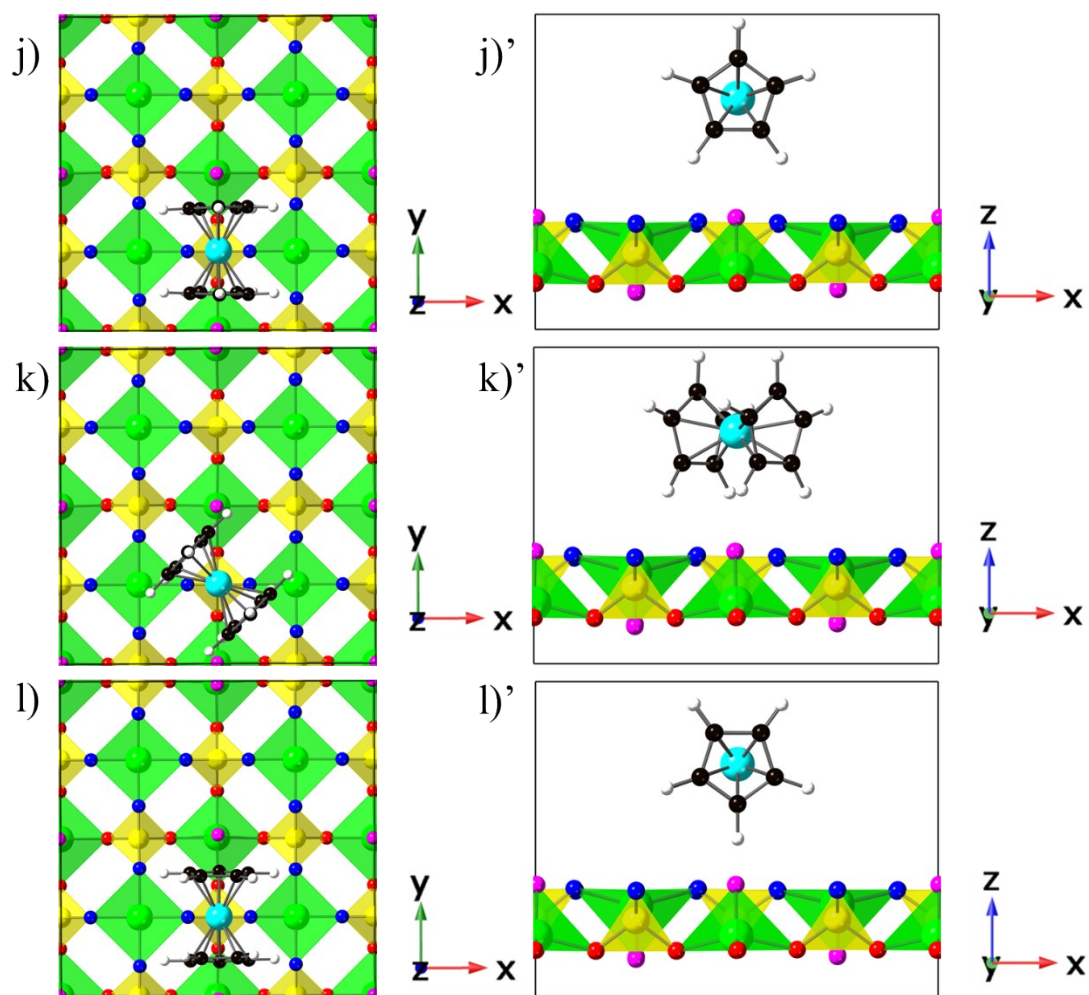


Figure S1. The configurations of j) E_{\perp} -P_{VO}-0°, k) E_{\perp} -P_{VO}-45°, and l) E_{\perp} -P_V-0° are viewed along the [001] direction. The corresponding pictures denoted with prime (') are viewed along the [010] direction. The black box is the unit cell.

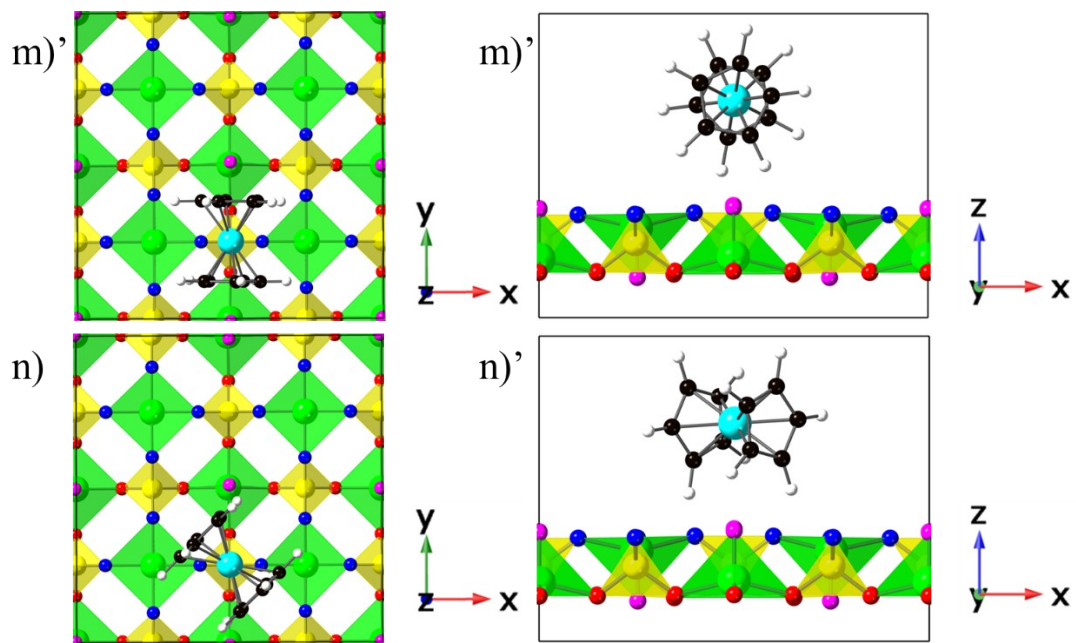


Figure S1. The configurations of m) S_1 -P- 0° and n) S_1 -P- 45° are viewed along the $[001]$ direction. The corresponding pictures denoted with prime (′) are viewed along the $[010]$ direction. The black box is the unit cell.

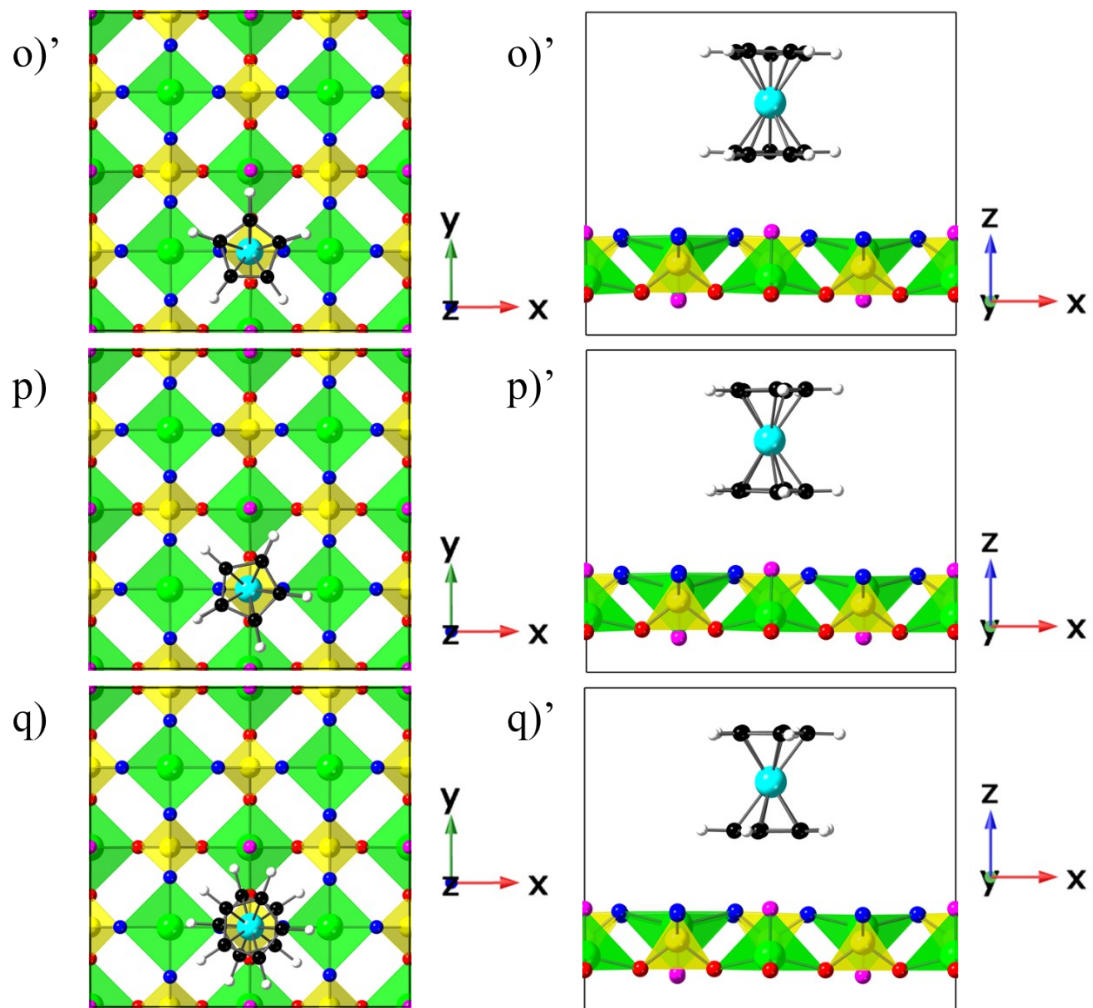


Figure S1. The configurations of o) E_{\parallel} -P- 0° , p) E_{\parallel} -P- 45° , and q) S_{\parallel} -P- 0° are viewed along the [001] direction. The corresponding pictures denoted with prime (') are viewed along the [010] direction. The black box is the unit cell.

The optimization of 14 structures.

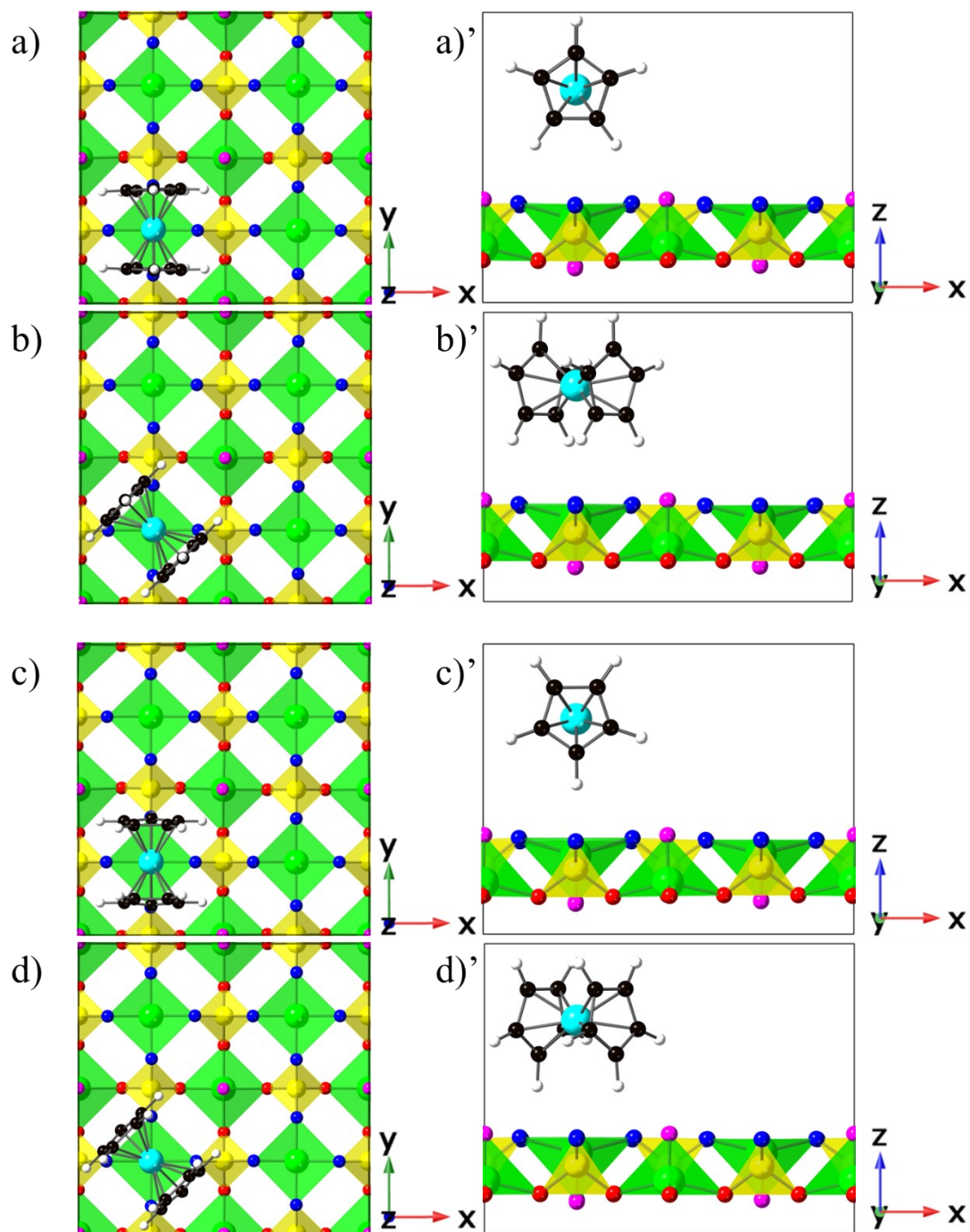


Figure S2. The configurations of a) E_{\perp} -VO-0°, b) E_{\perp} -VO-45°, c) E_{\perp} -V-0° and d) E_{\perp} -V-45° are viewed along the [001] direction. The corresponding pictures denoted with prime (') are viewed along the [010] direction. All subsequent configurations are shown in the same directions as these ones. The black box is the unit cell.

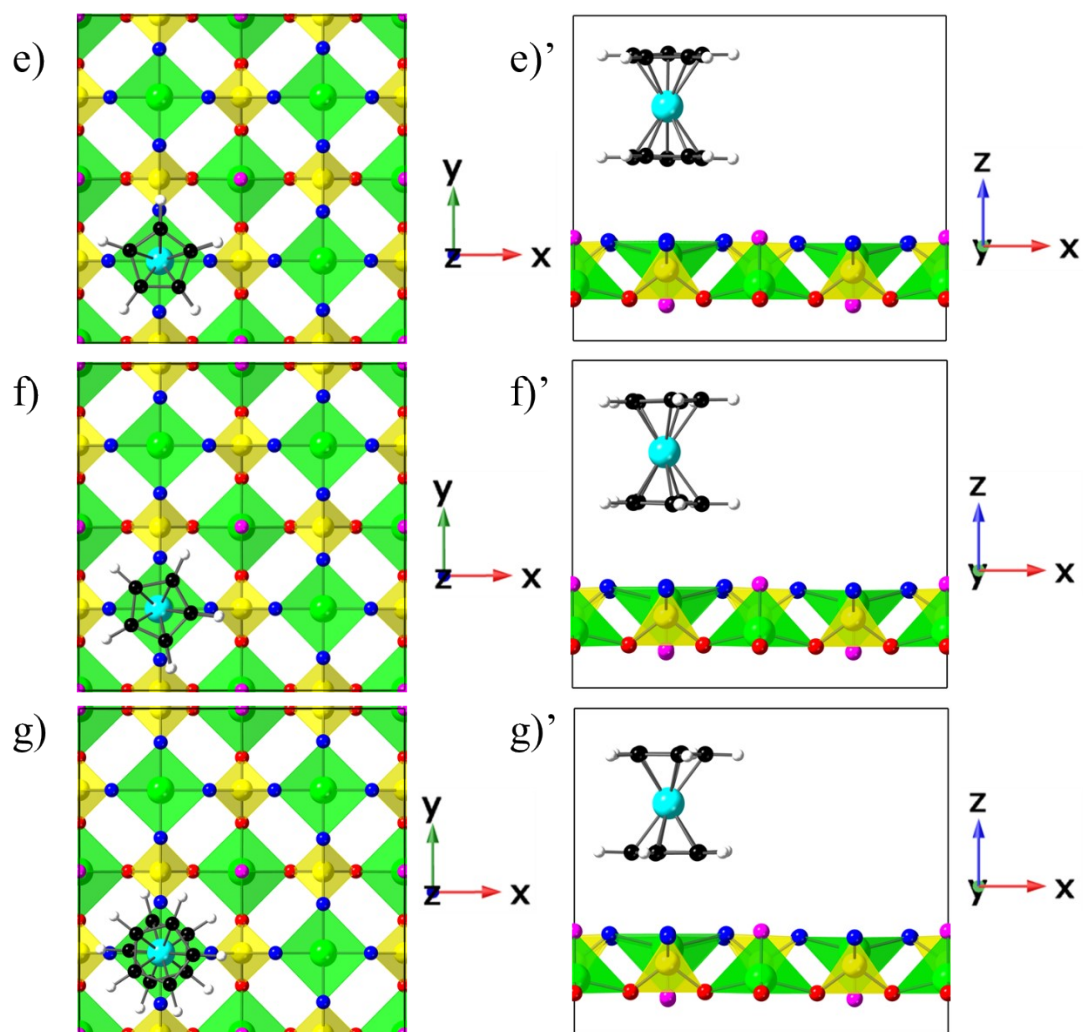


Figure S2. The configurations of e) $E_{\parallel}\text{-V-}0^{\circ}$, f) $E_{\parallel}\text{-V-}45^{\circ}$, and g) $S_{\parallel}\text{-V-}0^{\circ}$ are viewed along the $[001]$ direction. The corresponding pictures denoted with prime (') are viewed along the $[010]$ direction. All subsequent configurations are shown in the same directions as these ones. The black box is the unit cell.

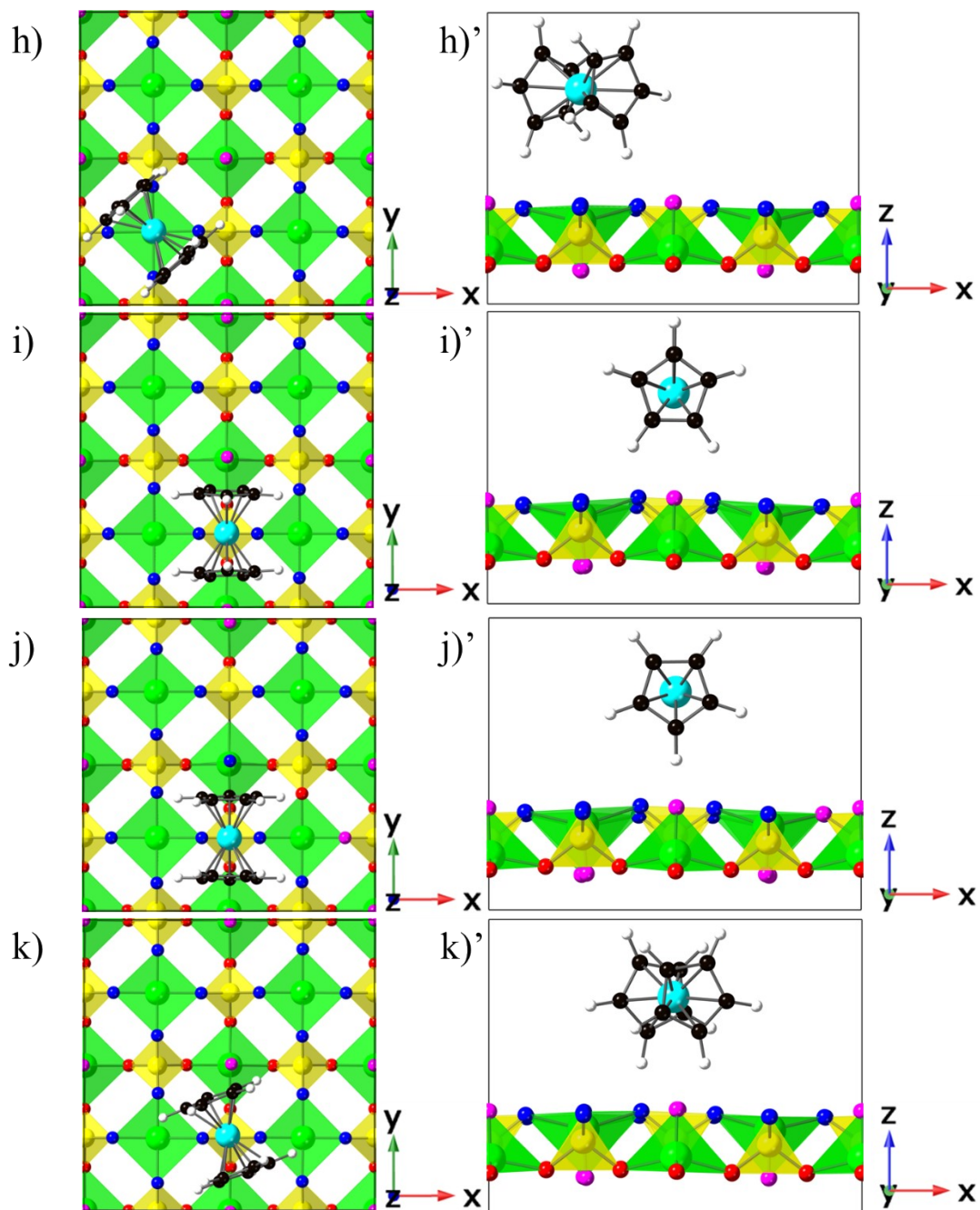


Figure S2. The configurations of h) $S_{\perp}\text{-V-}45^{\circ}$, i) $E_{\perp}\text{-P}_{\text{VO}}\text{-}0^{\circ}$, j) $E_{\perp}\text{-P}_{\text{V}}\text{-}0^{\circ}$ and k) $G_{\perp}\text{-P-}20^{\circ}$ are viewed along the [001] direction. The corresponding pictures denoted with prime (') are viewed along the [010] direction. The black box is the unit cell.

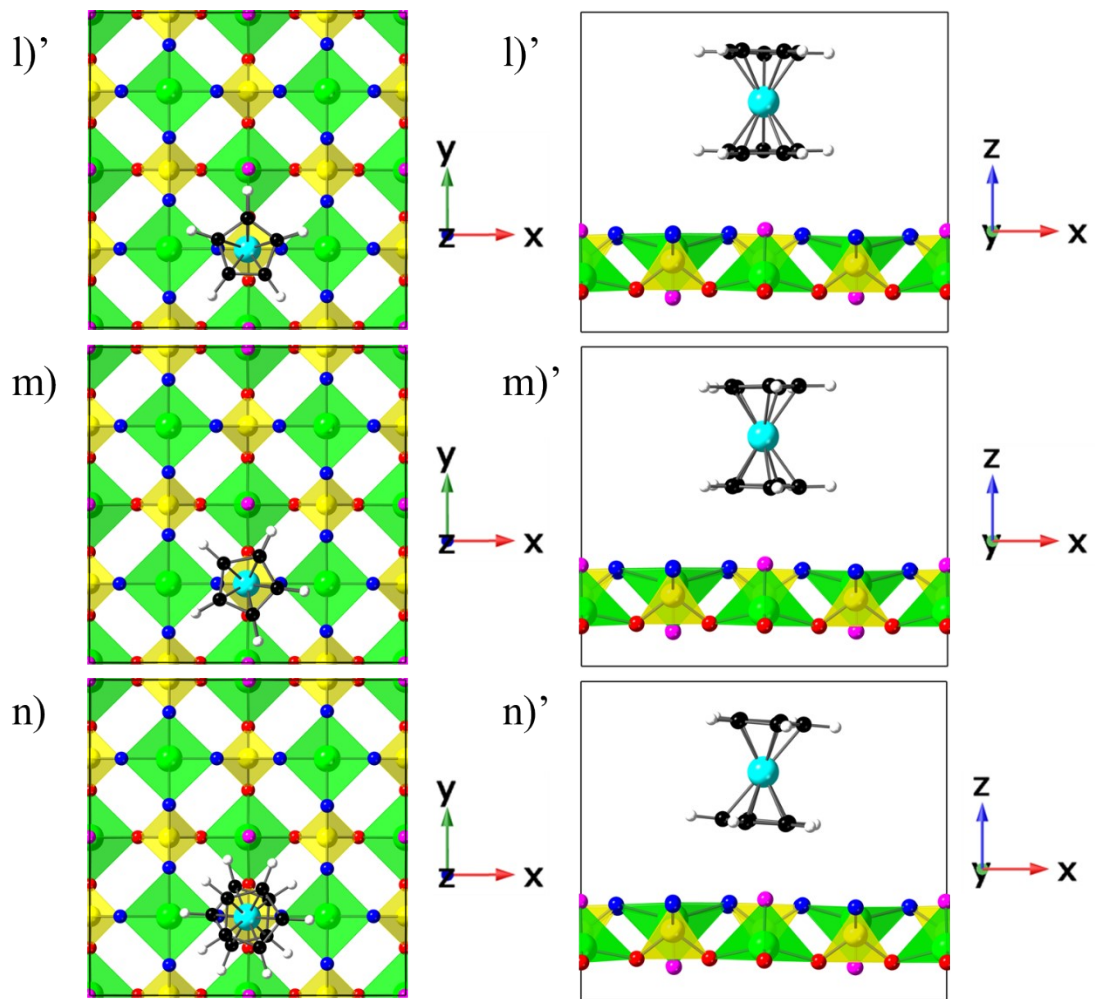


Figure S2. The configurations of l) $E_{||}\text{-P-}0^\circ$, m) $E_{||}\text{-P-}45^\circ$, and n) $S_{||}\text{-P-}0^\circ$ are viewed along the [001] direction. The corresponding pictures denoted with prime (') are viewed along the [010] direction. The black box is the unit cell.

The optimization of 14 structures parameters in POSCAR file.

E_{\perp} -VO-0°

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0.0000000000000000 12.4250515482596473 0.0000000000000000
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Direct

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O	P	V	C	H	Fe
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Direct

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$E_{\perp-V-0^{\circ}}$

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0.0000000000000000 12.4250515482596473 0.0000000000000000
0.0000000000000000 0.0000000000000000 9.7373736593534339

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Direct

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0.8500257145815624 0.0018196423365566 0.1340779966142733
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0.0021316218956855	0.1504502877070024	0.1347500816370513
0.9966446433054656	0.6502940326230799	0.1317848249922875
0.4976364862335245	0.1504905456954191	0.1347637457463691
0.5032081895025726	0.6503267644167607	0.1319634231362841
0.9985336616362588	0.7503807559302516	0.2267674540121050
0.0016509213402642	0.2503700059191090	0.2325949909486127
0.5012690372900366	0.7504153378431582	0.2269445100274439
0.4980619763230294	0.2503666117031003	0.2326951723163333
0.2498410376876663	0.9977350324047691	0.2240166101512742
0.2498826997730461	0.5029836570361326	0.2241498970387497
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0.0004537341343962	0.0003887667699232	0.1774332039743669
0.0005192307978206	0.5003134339948829	0.1775022885000794
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0.4993860232554539	0.5003508502305323	0.1777020575126542
0.2498939034483527	0.7503864645522853	0.2732396157551662
0.2497585550290111	0.2503923111708488	0.2708587611086344
0.7498934763050045	0.7504244308325525	0.2799413260454031
0.7498241282675835	0.2504289006759279	0.2771219744946123
0.3073941125663140	0.3780148790193394	0.8514961275409476
0.1929251220515980	0.1232904467269265	0.8498865993373386
0.3440525803589054	0.3906370295319590	0.7129333966915326
0.2521375062000715	0.3992864227235700	0.6265523548107836
0.1582306383229621	0.3903864222655713	0.7093739973765949
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0.2519125384361800	0.1022985919678163	0.6264397820002898
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0.1420997125752379	0.1339088243727034	0.9393193833505080
0.3585764642622848	0.1347159252098535	0.9409689285966891
0.4272725450124284	0.1114139191015298	0.6761215361971082
0.3567380984721993	0.3672366112922418	0.9422084136257922
0.1402863911448904	0.3669189036106459	0.9381810545609923
0.2523749272901199	0.0944107620899075	0.5154510684984146
0.2533529248125319	0.4071651450586273	0.5155719338757407
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S_I-V-45°

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0.8972614630658288	0.2493454751463639	0.3250778974689453
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0.5998999143665135	0.7488638348472737	0.3266568868177317
0.6032063066782732	0.2510944258064655	0.3310431593510185
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0.2482668041183221	0.4038232816725949	0.3326410504646390
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0.5000735561213808	0.8498032397254182	0.1369064687194394
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0.2224153049093345	0.0397815897778510	0.6372105473210340
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0.4293497047703478 0.3041006183743398 0.8806445506028495
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0.1409906898375186 0.1016551410192572 0.8694820286324108
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0.2560115686873010 0.4342890719060454 0.8853611065643223
0.0777791804996448 0.3104116219949289 0.8779630847061344
0.0760755915317907 0.3094253532895845 0.5644827759770547
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E_{\parallel} -V-45°

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0.0000000000000000 12.4250515482596473 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.8465968913686392

O P V C H Fe
40 8 8 10 10 1

Direct

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0.8964669084056496 0.2495595158552604 0.2991338781262129
0.2501069179309923 0.7501537186932481 0.1089578805770586
0.2499486458803375 0.2495098376581808 0.1161621480330481
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0.9997536019414355 0.5001584445815297 0.3158404825871344
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0.0939075452781921 0.2494426061702200 0.3075821904814333
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0.2501372038970118 0.4056798389401806 0.3074245925579007
0.7498650976457242 0.8994242531380721 0.2971899441800971
0.7499227357344154 0.4001610986947171 0.2969552414723395
0.9996964500644623 0.8500847232068409 0.1266700251141586
0.9995031935424592 0.3494097817099373 0.1305462782683477
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0.2500195313865774 0.4993740451181097 0.2178280894360185
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0.0005953498364448 0.4990749565206443 0.1692284914162201
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$S_{\parallel-V-0^\circ}$

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0.0000000000000000 12.4250515482596473 0.0000000000000000
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O P V C H Fe
40 8 8 10 10 1

Direct

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0.7514179883966590	0.6005782692470524	0.2924042638593446
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0.4062093901108753	0.2504947464423814	0.3066330482331393
0.9007170975104392	0.7506141690609028	0.2898545124366378
0.8981031836179988	0.2504020654750324	0.2939390059171801
0.2536304613719655	0.7501478441676199	0.1087591337643865
0.2545301123988713	0.2505943741186842	0.1054289440399934
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0.7507573912655456	0.2505548674545837	0.1041628345638211
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0.5040641354622052	0.9975193002363447	0.3164170769815108
0.5042710286588864	0.5037804984833363	0.3172729150423066
0.1000826083702998	0.7504607239650433	0.2909024339688228
0.0963890191104309	0.2501931707564506	0.3006886802658651
0.6020441370790385	0.7504767179186087	0.2958109501630600
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0.2512747480985518	0.8971786714138917	0.2999112827653114
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0.7524520855337531 0.2504308130052716 0.2509991401622161
0.5376885361053128 0.1518139758248936 0.8653262643151087
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E_l-P_{vo}-0°

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O P V C H Fe
40 8 8 10 10 1

Direct

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0.0008309493300881	0.4996446356894554	0.1899845868771580
0.4993577805188803	0.9981466808048127	0.1976865967375517
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0.2497912198311452	0.7504105760310391	0.2912976543565739
0.2520303730555642	0.2504265135302658	0.2947734827998583
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0.7507818859963595	0.2505037660218339	0.2906167688362645
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0.4427078699637065	0.3979937003236631	0.6283117786197805
0.5954758849729515	0.1211361956065144	0.7651448592703394
0.5029816417102030	0.1257082331334917	0.8534770050360483
0.4088603336046701	0.1170306533087491	0.7688327570295621
0.4433160338590879	0.1062717478887032	0.6297373303349212
0.5571529065957567	0.3961145364137024	0.6272623161069155
0.5938453908236979	0.3851125844660294	0.7658873114333261
0.5006484997156910	0.3797780210060018	0.8529409024628107
0.4071685688980353	0.3872601449555736	0.7669758027463697
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0.5007161809115995	0.3659695520901036	0.9627882201546671
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E₁-P_V-0°

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12.4250515482596473 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.4250515482596473 0.0000000000000000
0.0000000000000000 0.0000000000000000 9.7373736593534339

O P V C H Fe
40 8 8 10 10 1

Direct

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E_{||}-P-45°

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Direct

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The Total Energy comparison.

Table S2. The relative total energy of 17 different configurations. The reference is E_{\perp} -V-45°. Unit in eV.

V/VO	0°	45°
E_{\perp} -VO	+0.063	+0.065
E_{\perp} -V	+0.176	0
S_{\perp} -V	+0.061	+0.050
E_{\parallel} -V	+0.538	+0.537
S_{\parallel} -V		+0.558
P/P	0°	45°
S-P	+0.084	+0.082
E-P _{VO}	+0.208	
E-P _V	+0.122	+0.084
E_{\parallel} -V	+0.612	+0.625
S_{\parallel} -V		+0.617

The comparison of Gibbs Free Energy of E_{\perp} -V-45° and S_{\perp} -V-45°

The vibrational calculations are conducted using the IBRION=6 setting in the INCAR file. Subsequently, frequency information is extracted utilizing the function 501 in VASPKIT.¹

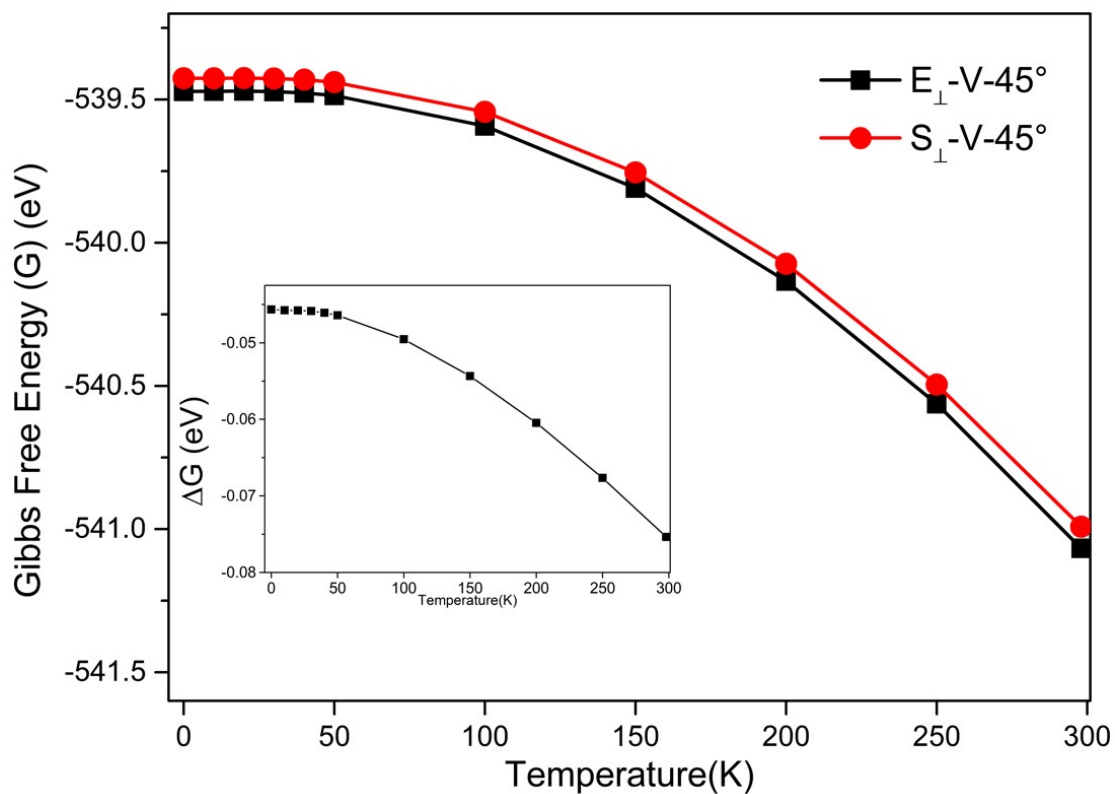


Figure S3. The Gibbs Free Energy variations as a function of temperature for the E_{\perp} -V-45° (in black) and S_{\perp} -V-45° (in red) configurations. An inset detail provides a focused comparison of the differential Gibbs Free Energy between these configurations across varying temperatures.

The Bader Charge Analysis.

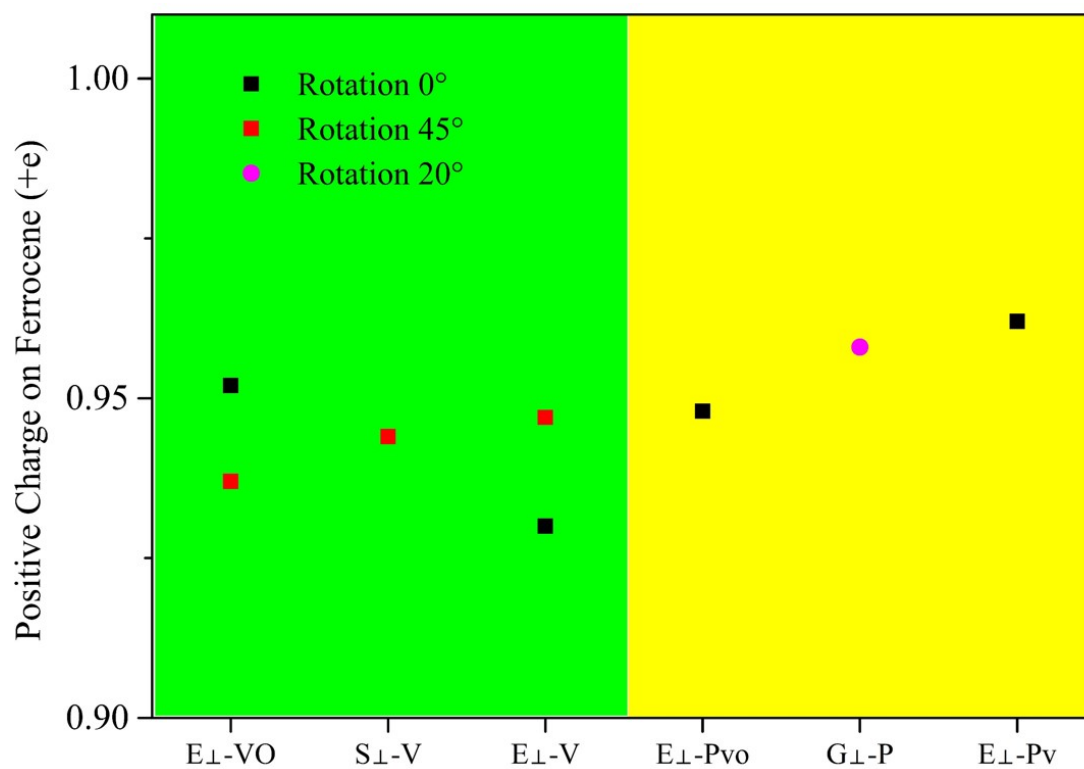


Figure S4. Bader charges analysis of eight unique configurations and compared them with experimental data.² The green region means the ferrocene located on V/VO site, while yellow region means the ferrocene located on P/P site.

The charge density difference maps of eight different configurations.

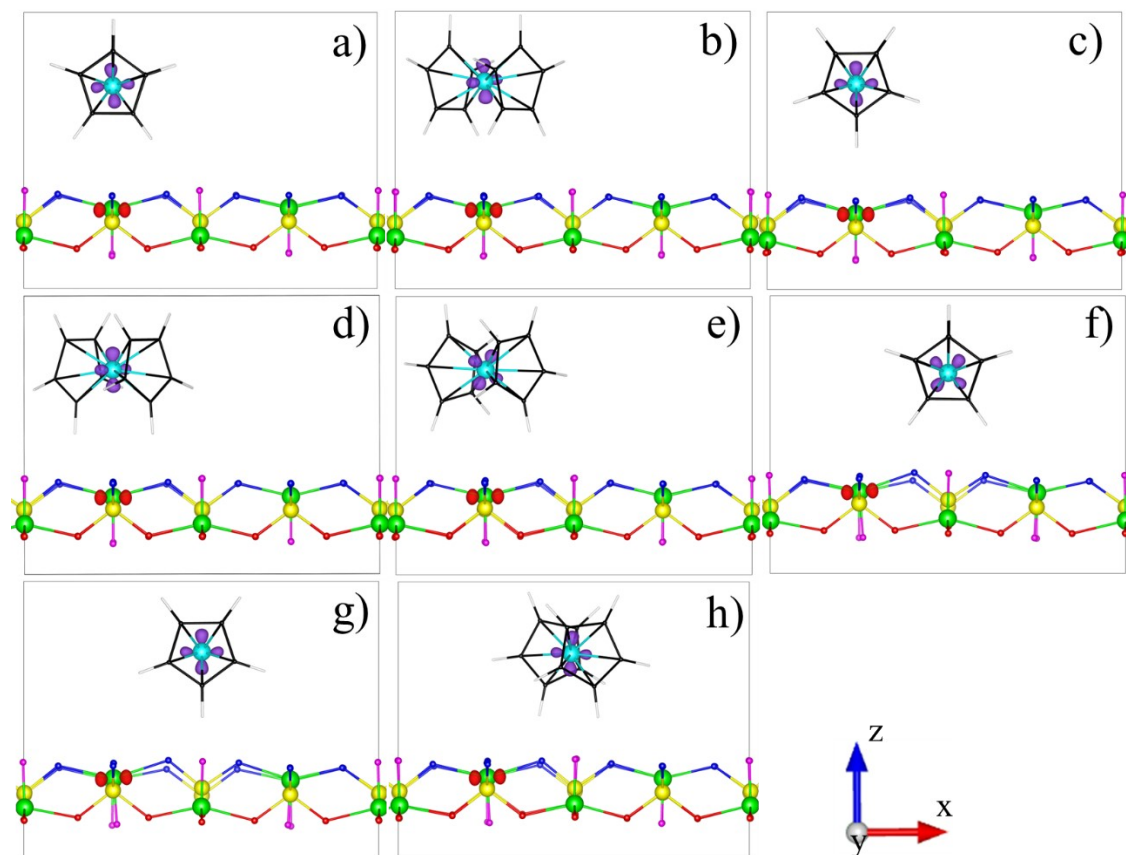


Figure S5. The charge density maps of a) E_{\perp} -VO- 0° , b) E_{\perp} -VO- 45° , c) E_{\perp} -V- 0° , d) E_{\perp} -V- 45° , e) S_{\perp} -V- 45° , f) E_{\perp} -P_{VO}- 0° , g) E_{\perp} -P_V- 0° , and h) G_{\perp} -P- 20° . The red region means the charge accumulation, while the violet region means the charge reduction. The issovalue is $0.04 \text{ e}/\text{\AA}^3$. All of pictures viewed along $[010]$ direction. The black box is the unit cell.

The charge density difference when ferrocene intercalated on P/P site.

When ferrocene is intercalated at the P/P site, four possible sites for charge accumulation on the vanadium are observed. These sites are labeled as V_Top, V_Bottom, V_Left, and V_Right, as illustrated in Figure S3. From a symmetry perspective, V_Top is equivalent to V_Bottom, while V_Left is equivalent to V_Right.

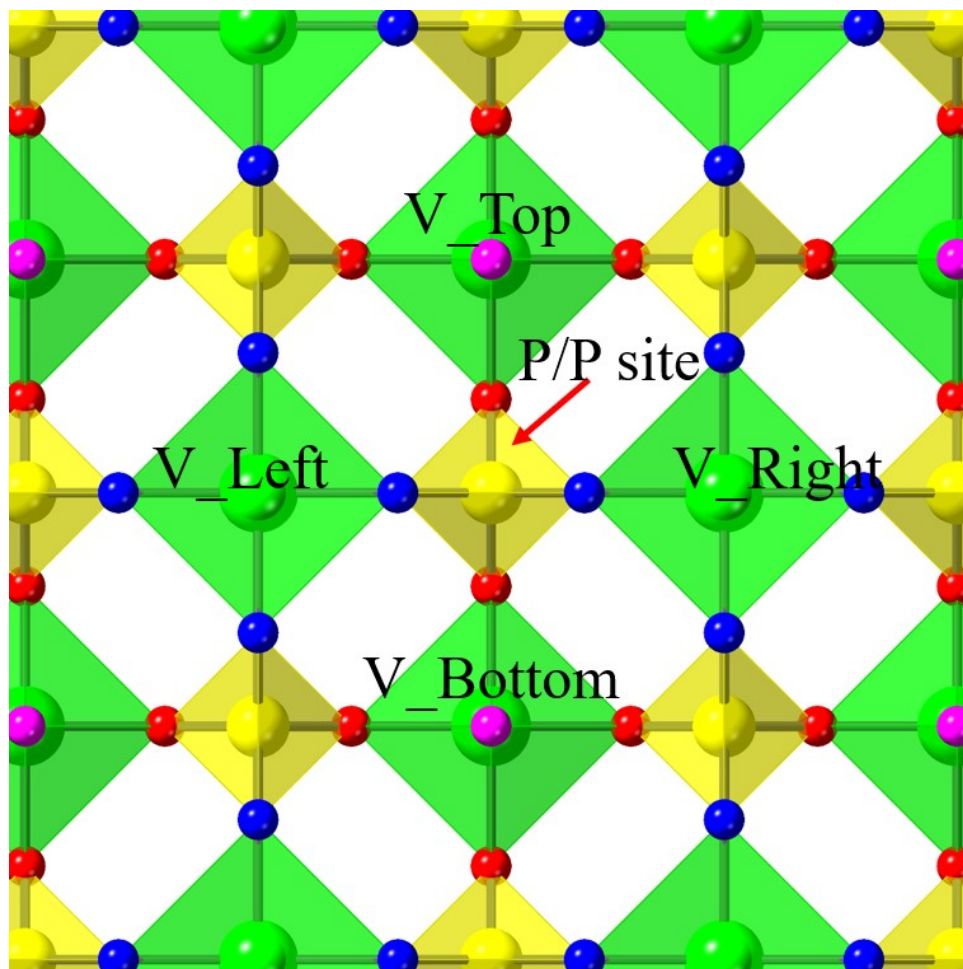


Figure S6. The four possible charge accumulations of vanadium.

Table S3. The Relative total energy of four possible charge accumulation of vanadium. The reference is the charge accumulation on the left. Unit in eV.

Charge Accumulation	Relative total energy (eV)
V_Left	0
V_Right	+0.003
V_Top	+0.040
V_Bottom	+0.041

The 2D charge density difference map of G_{\perp} -P-20° along [001] direction.

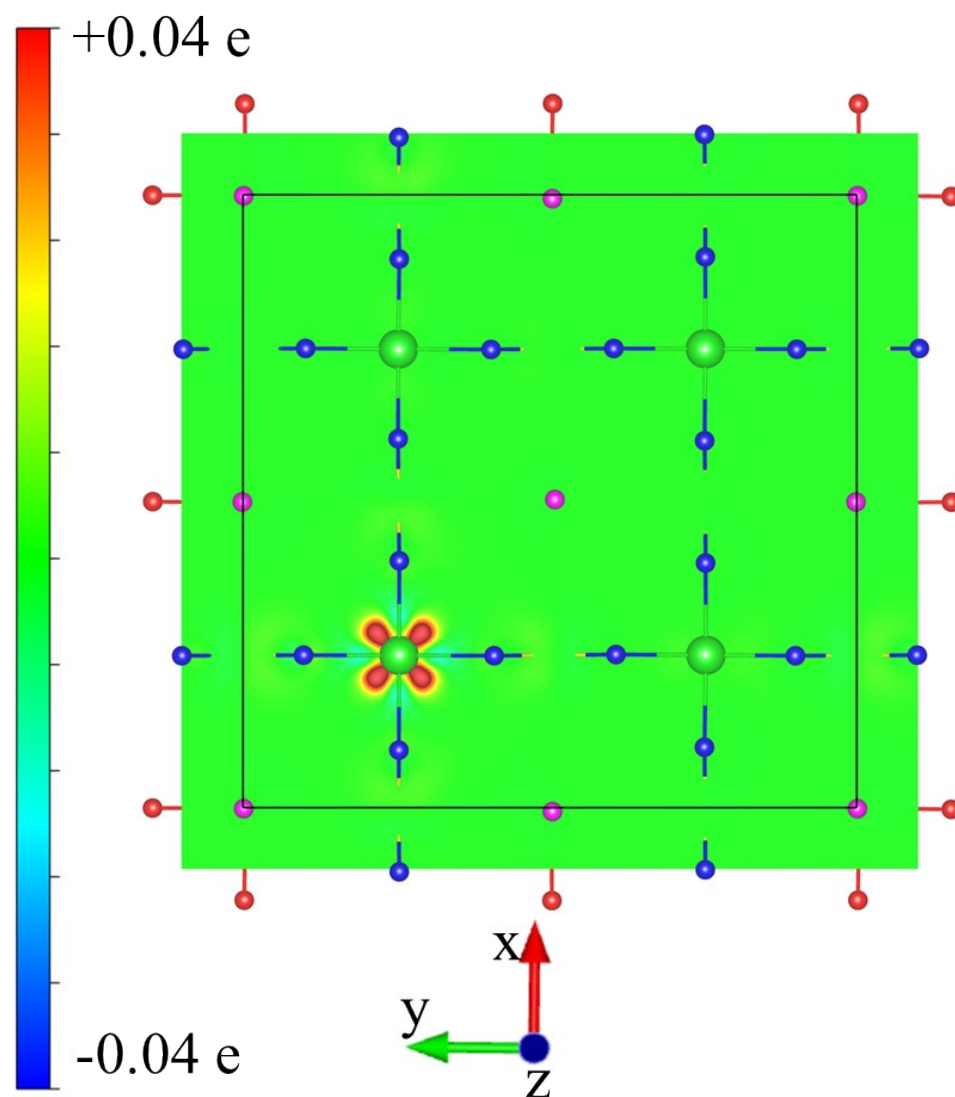


Figure S7. The charge density difference map built by the four vanadium atoms, viewed along [001] direction; the ferrocene has been omitted due to the clarity. The red region means the charge accumulation. The black box indicated the unit cell. The iso-value is $0.04 \text{ e}/\text{\AA}^3$.

The dihedral angle of ferrocene with and without D3 calculations.

Table S4. The dihedral angle of ferrocene with and without D3 calculations.

Dihedral Angle (°)	With D3	Without D3
E₁-VO-0° Ferrocene	2.98	2.99
E₁-VO-45° Ferrocene	2.34	2.77
E₁-V-0° Ferrocene	13.49	13.78
E₁-V-45° Ferrocene	12.04	12.54

The charge density difference of supercell structure.

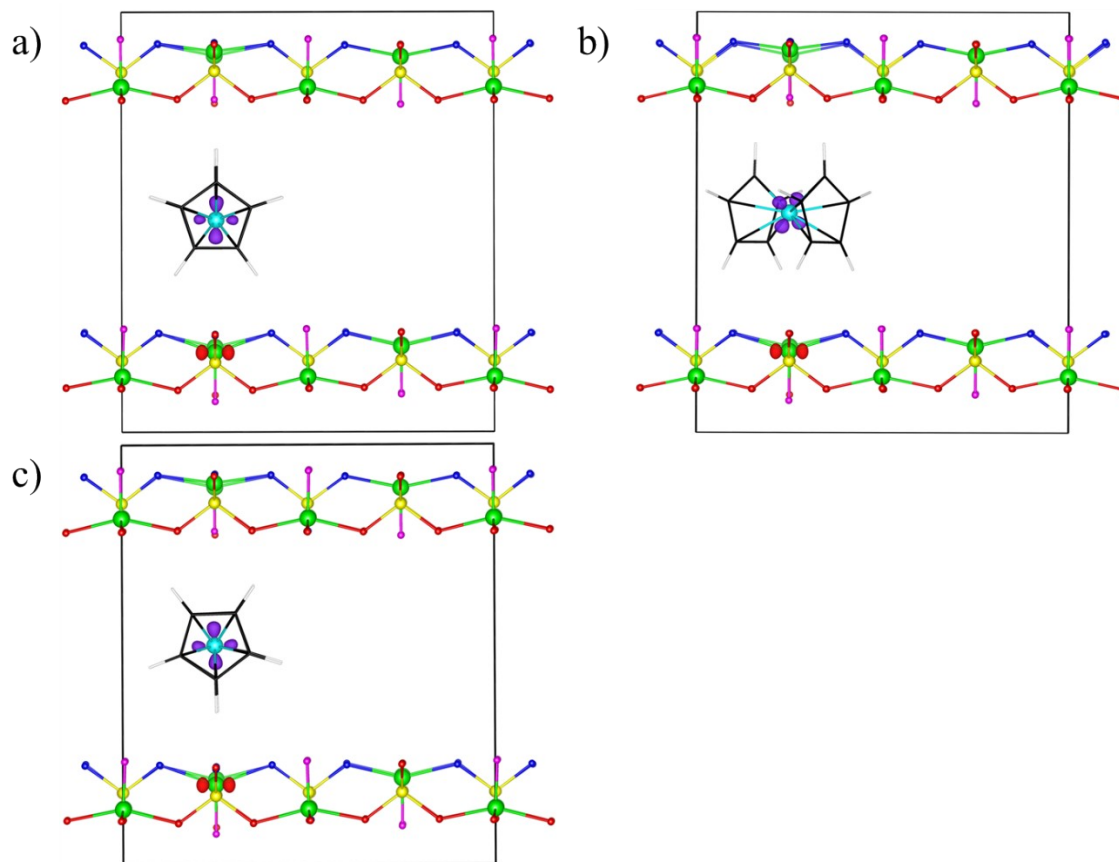


Figure S8. The charge density difference map of a) E_{\perp} -VO- 0° configuration, b) E_{\perp} -VO- 45° and c) E_{\perp} -V- 0° , the violet region is the charge reduction and red region is the charge accumulation, the iso-value is $0.04 \text{ e}/\text{\AA}^3$, viewed along [010] direction. The black box is the supercell structure.

The Hirshfeld surface analysis.

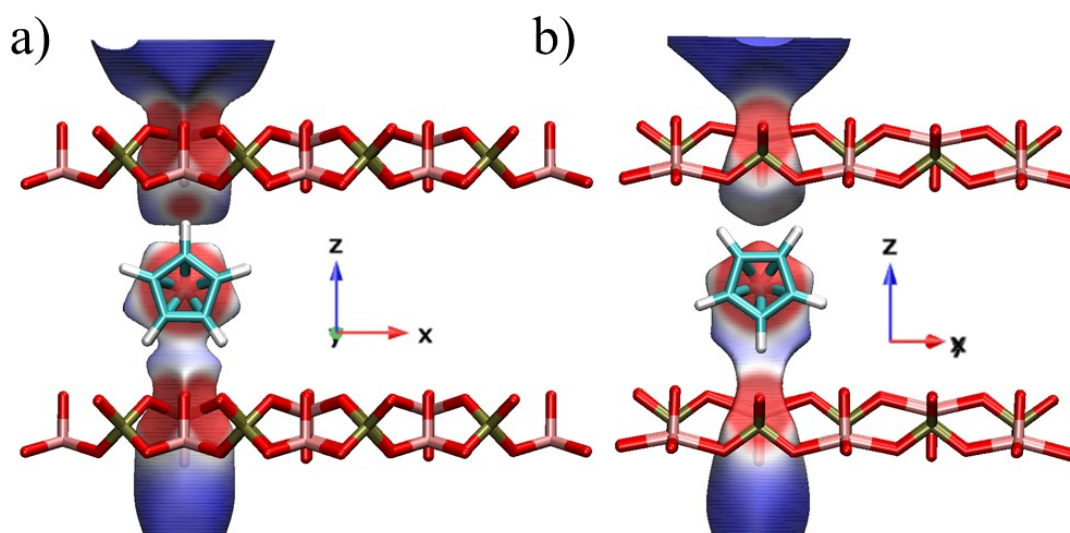


Figure S9. The Hirshfeld surface analysis of a) E_{\perp} -VO-45°, viewed along [010] direction, and b) E_{\perp} -V-0°, viewed along [-110] direction. Red means high electron density, white means medium electron density and blue means low electron density

The other orientation of Hirshfeld surface analysis.

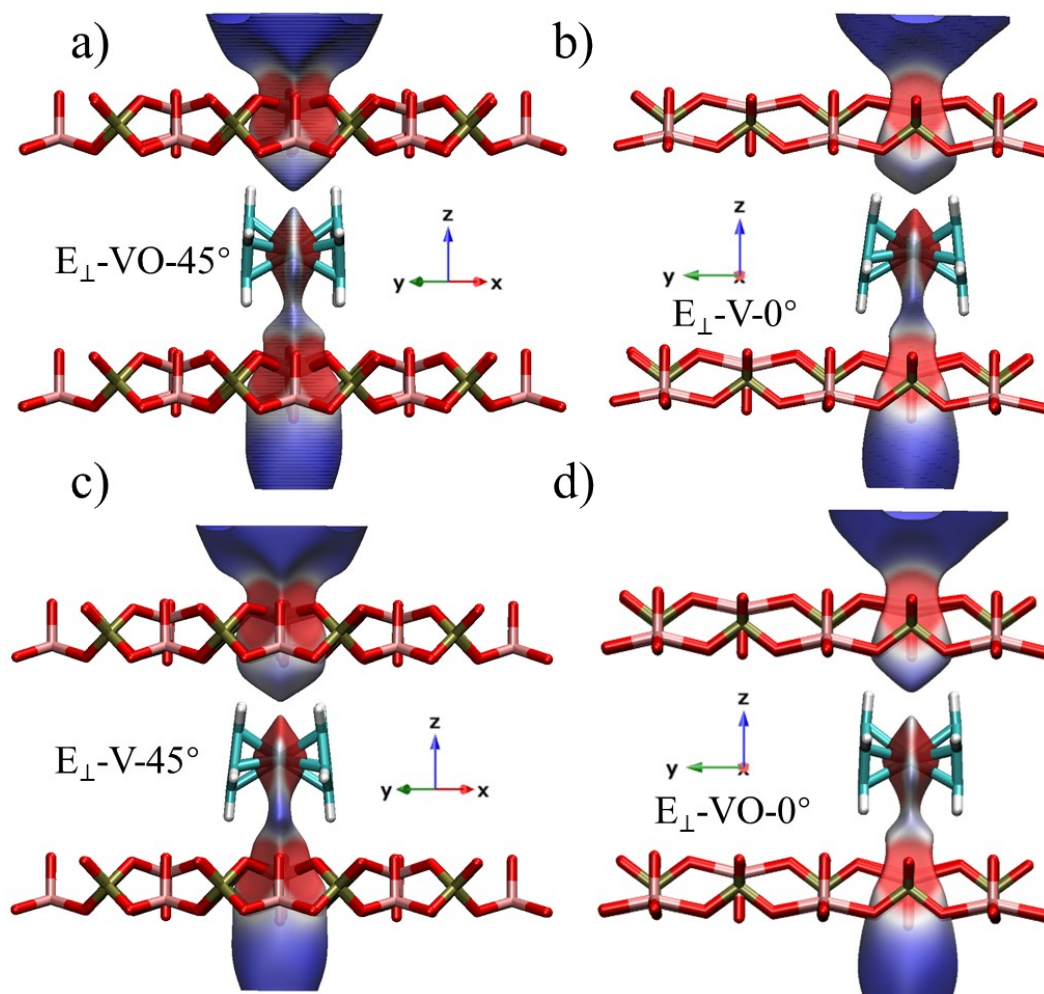


Figure S10. The Hirshfeld surface analysis of a) E_{\perp} -VO-45°, viewed along [110] direction, b) E_{\perp} -V-0°, viewed along [100] direction, c) E_{\perp} -V-45°, viewed along [110] direction, and d) E_{\perp} -VO-0°, viewed along [100] direction.

Reference.

- 1 V. Wang, N. Xu, J.-C. Liu, G. Tang and W.-T. Geng, *Comput. Phys. Commun.*, 2021, **267**, 108033.
- 2 A. Davidson, G. Villeneuve, L. Fournes and H. Smith, *Mater. Res. Bull.*, 1992, **27**, 357–366.