

Supporting Information for

Role of proton on enhanced Mg^{2+} migration in $\alpha\text{-V}_2\text{O}_5$ cathode for magnesium battery: A first-principle investigation

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1) The Bader charge of the $\alpha\text{-V}_2\text{O}_5$ systems

Table S1. Bader charge (in electrons) of $\alpha\text{-V}_2\text{O}_5$, $\text{Mg}_{0.25}\text{V}_2\text{O}_5$, and $\text{Mg}_{0.25}\text{H}_2\text{V}_2\text{O}_5$. The first line gives the total charge of the corresponding atom, while the second line (with “+” or “-” signs) gives the obtained (+) or lost (-) charge of the corresponding atom.

V_2O_5		$\text{Mg}_{0.25}\text{V}_2\text{O}_5$			$\text{Mg}_{0.25}\text{H}_2\text{V}_2\text{O}_5$			
O	V	O	V	Mg	O	V	Mg	H
6.63	8.87	6.89	8.88	6.25	7.32	9.02	6.25	0.36
+0.63	-2.13	+0.89	-2.12	-1.76	+1.32	-1.98	-1.75	-0.64

2) The energy profile for Mg-ion migration along the b-axis direction in $H_xV_2O_5$.

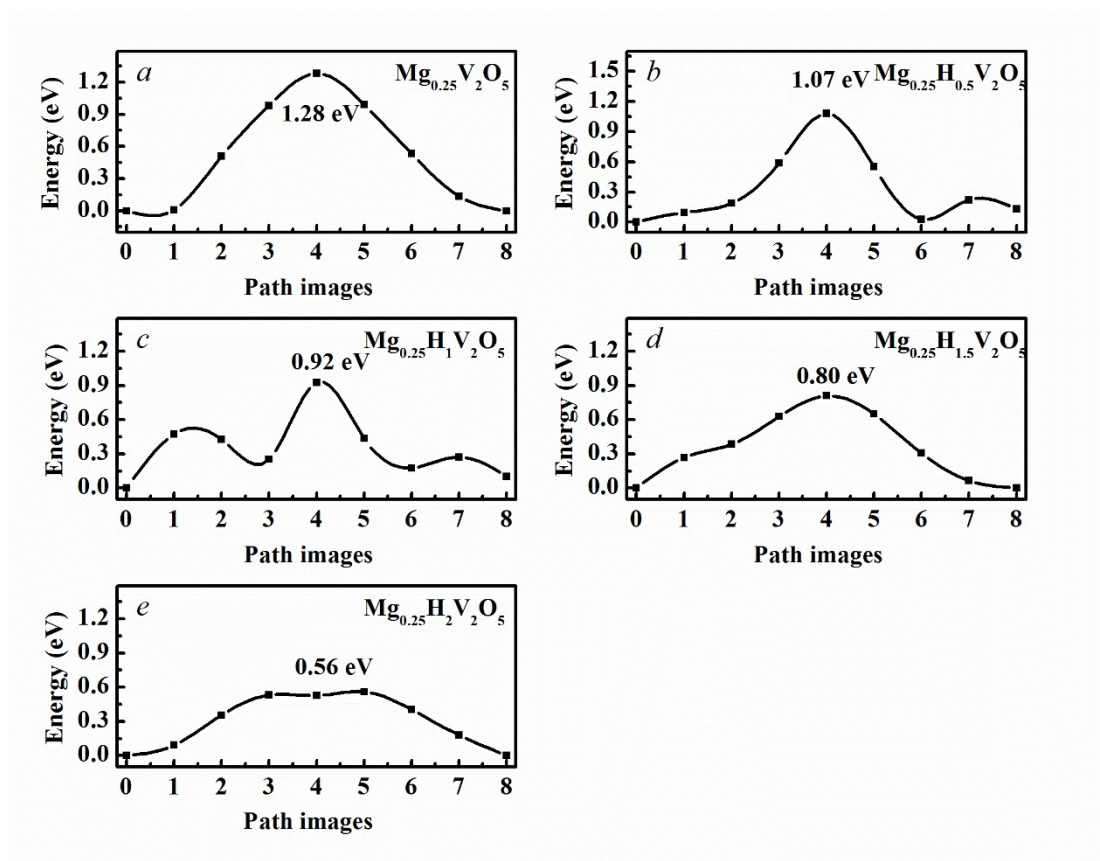


Fig. S1. The energy profiles for Mg-ion migration along the b-axis direction in $H_xV_2O_5$ for (a) $x=0$, (b) $x=0.5$, (c) $x=1$, (d) $x=1.5$, and (e) $x=2$.

3) The INCAR file we used and relaxed structures (CONTCAR files)

INCAR file

Start parameter for this run:

```
SYSTEM = H2V2O5
NWRITE =      2
ISTART =      0
ICHARG =      2
ISPIN  =      2
INIWAV =      1
ENCUT  = 520.0 eV
NELM   =     120
NELMIN =      8
EDIFF  = 1.0E-05
LREAL  =      A
EDIFFG =  -0.01
NSW    =     200
IBRION =      2
ISIF   =      3
ISMEAR =      0
SIGMA  =   0.05
```

NEDOS = 1000

```
LVDW = .TRUE.
VDW_RADIUS = 30.00
VDW_SCALING = 0.75
VDW_D = 20.0
LDAU = .TRUE.
LADUTYPE = 2
LDAUU = 3.0  0.0  0.0
LDAUJ = 1.0  0.0  0.0
LDAUPRINT = 0
LMAXMIX = 4
LWAVE =      T
LCHARG =      T
LORBIT =     11
LPLANE = .TRUE.
NPAR = 4
LSCALU = .FALSE.
NSIM = 4
```

IMAGES=7

SPRING=-5

The relaxed CONTCAR files

1. V₂O₅

```

                                CONTCAR
1.0000000000000000
11.6417999267999992    0.0000000000000000    0.0000000000000000
  0.0000000000000000    7.1476001739999999    0.0000000000000000
  0.0000000000000000   -0.0000000000000000    4.4320001600000003
V      O
  8      20
Direct
0.1012599989999998    0.1249900010000005    0.8825600150000028
0.3987399940000032    0.1249900010000005    0.8825600150000028
0.8987399940000032    0.3749899860000028    0.1174400000000020
0.6012600059999968    0.3749899860000028    0.1174400000000020
0.1012599989999998    0.6249899860000028    0.8825600150000028
0.3987399940000032    0.6249899860000028    0.8825600150000028
0.8987399940000032    0.8749899860000028    0.1174400000000020
0.6012600059999968    0.8749899860000028    0.1174400000000020
0.1032200009999968    0.1249900010000005    0.5197299720000004
0.9313300250000012    0.1249900010000005    0.0065700000000035
0.3967800140000008    0.1249900010000005    0.5197299720000004
0.5686600209999995    0.1249900010000005    0.0065700000000035
0.0686599980000011    0.3749899860000028    0.9934300179999980
0.8967800140000008    0.3750000000000000    0.4802699979999971
0.4313400090000030    0.3749899860000028    0.9934300179999980
0.6032199859999992    0.3750000000000000    0.4802699979999971
0.2500000000000000    0.1249900010000005    0.9897199870000009
0.7500000000000000    0.3749899860000028    0.0102800000000016
0.1032200009999968    0.6249899860000028    0.5197299720000004
0.9313300250000012    0.6249899860000028    0.0065700000000035
0.3967800140000008    0.6249899860000028    0.5197299720000004
0.5686600209999995    0.6249899860000028    0.0065700000000035
0.0686599980000011    0.8749899860000028    0.9934300179999980
0.8967800140000008    0.8750000000000000    0.4802699979999971
0.4313400090000030    0.8749899860000028    0.9934300179999980
0.6032199859999992    0.8750000000000000    0.4802699979999971
0.2500000000000000    0.6249899860000028    0.9897199870000009
0.7500000000000000    0.8749899860000028    0.0102800000000016

```

2. $\text{H}_{0.5}\text{V}_2\text{O}_5$

CONTCAR

```

1.0000000000000000
  11.9230378758491824    0.0017521933248925    0.0025533111154966
 -0.0288016571375592    7.2500699885241549   -0.0006451297786645
   0.0045141659057151   -0.0055653798098142    4.1260632957699679
V      O      H
  8     20     2
Direct
0.1048115237901090  0.1228653152578872  0.8926198381540009
0.3993795652383288  0.1181636596153862  0.8983748484832512
0.9068531719246111  0.3699088907600401  0.1148369828703898
0.6085590424721778  0.3720884302371877  0.0567003782933111
0.0954828190145587  0.6245760566378954  0.8890141436239509
0.3921928569688360  0.6159508998232197  0.9893302134154084
0.9022155069371117  0.8745669897993567  0.0996662637215842
0.6080217420665176  0.8741701218724182  0.0826660297308489
0.1049720372588273  0.1238158377538432  0.5013947408407630
0.9366117621827141  0.1169242714712513  0.9977524436274495
0.3996487320219705  0.1190770044545299  0.5051171604320286
0.5755708489975960  0.1227630389952187  0.9849697633243616
0.0725668622634264  0.3733889276635542  0.9973452937432979
0.9004260011942495  0.3718471507376496  0.5085293011783668
0.4341564994455946  0.3648877352290385  0.0005951247418637
0.5895634456607437  0.3894060120950026  0.4961088346889802
0.2516027183971642  0.1205472411262397  0.9912879617026168
0.7501392410559451  0.3676755209843575  0.0335185023999874
0.1030175645336462  0.6230973004759479  0.4987032743983097
0.9352456366501426  0.6267607344354802  0.9935519046722333
0.4170160855261327  0.6265383873809895  0.4983970638530308
0.5728607112951543  0.6230519988754140  0.9950450569249000
0.0734850354481849  0.8726190704931522  0.9949797848233902
0.9000832188276314  0.8722496178055565  0.4910640631551954
0.4368708137178952  0.8758849841241053 -0.0017953028836495
0.6026448773678214  0.8716206396424906  0.4794139864242966
0.2486189830072704  0.6251493154070497  0.9910466188065004
0.7536627729818866  0.8734588050093505  0.9984202046728465
0.5188813759677608  0.4673132976964186  0.5081239794388214
0.4623987827860114  0.7411722851399835  0.5026719627416463

```

3. HV₂O₅

CONTCAR

1.0000000000000000

12.0681329511671436	-0.0070022930978073	-0.0471807234568304
-0.0045169305866447	7.2998934913451956	-0.0010657859968924
-0.0099729564734639	-0.0004080952864733	4.0525058300223895

V	O	H
8	20	4

Direct

0.0997655015973920	0.1237286527617884	0.8995083886505080
0.3919058665017992	0.0895973069757391	-0.0029453485242929
0.9027486242892480	0.3729342467339763	0.1018487303672164
0.6102142229843888	0.3395845890582498	0.0028303372222631
0.0976004518256558	0.6251479126113961	0.8991462788431731
0.3899320573654264	0.5887397215918181	-0.0020271352101713
0.9002764555115926	0.8742194709261762	0.1020134308438390
0.6078613955068375	0.8400037453340677	0.0050316982705241
0.0983136286153273	0.1251256321760652	0.4994132870028719
0.9328161846743074	0.1235795440962219	0.0067536076756754
0.4123870372269876	0.1100255131895676	0.4992181329215017
0.5709266832941161	0.0994439054681764	0.0020802609731011
0.0661517651491743	0.3737748627307583	-0.0035326790084791
0.9005984612383278	0.3743501042183941	0.5010150162758716
0.4307944483664530	0.3508377024858532	-0.0010794909721845
0.5872059978529190	0.3576090794540619	0.5018018638207963
0.2436348615221881	0.1215503792658029	-0.0035452574962613
0.7553435916205598	0.3678250998704646	0.0042494682371300
0.0988551388831804	0.6245687441156870	0.4997551126597328
0.9335137340239484	0.6224641172224180	0.0051949524004000
0.4134479075816852	0.6068712191009773	0.4996712690655349
0.5718420541285636	0.6030147436574954	0.0022364167804284
0.0682990305718963	0.8727897505991599	0.9946362379179667
0.9028907281057091	0.8740286939698197	0.5021944408360366
0.4268933998725707	0.8514082828049253	-0.0008627062834645
0.5866091909482292	0.8597726557003970	0.5029109960121001
0.2443894384360318	0.6148191948020001	-0.0031233923306891
0.7570421775122230	0.8671911344312249	0.0054052259639831
0.4662492324866787	0.7120182486558655	0.5014802880696504
0.5322534997416306	0.9624572642095000	0.5010676903043002
0.5339488070947099	0.4620592357376795	0.4999509310240277
0.4674385144702545	0.2119490290443143	0.5006218866869308

4. $\text{H}_{1.5}\text{V}_2\text{O}_5$

POSCAR

```

1.0000000000000000
12.2766859383831992    0.0059729567344658    -0.0135595106251628
0.0033382705210228    7.3483104425024726    0.0059760870847194
0.0045537496085568    0.0041630080761686    4.0006978912110682
V      O      H
8      20     6
Direct
0.1009578405228246    0.1555039449870386    -0.0056499470368462
0.3912807264020682    0.1498297893871046    -0.0039252870819933
0.8992422198310114    0.3865907628632846    0.0777285946723121
0.6101178309061859    0.4044496902535366    -0.0063594108764125
0.1026015839112023    0.6569517157935154    -0.0021105414101753
0.3929812455184009    0.6473389775430097    -0.0041749335117458
0.8919234118030862    0.8865751869749305    0.0757358888660079
0.6020661178238049    0.9029553972965797    -0.0016744578886743
0.0879498123039023    0.1259505950111945    0.4985770571602374
0.9270471088744970    0.1430300631566648    -0.0046214096715766
0.4209194889945753    0.1338012486965842    0.4951667898697554
0.5811629540943580    0.1401191104687947    -0.0036055127803087
0.0601537037220662    0.3991733460657081    0.0022542939263113
0.8990664189313166    0.3947664756763984    0.4879377932001283
0.4339125561743706    0.3888755471751262    -0.0056747913082538
0.5856194676805377    0.3837922733816965    0.4940089610999347
0.2529185832601982    0.1628721619567920    -0.0040391358303068
0.7524482165041174    0.3947718250172925    -0.0086969822335905
0.0908890945779578    0.6275978314483911    0.5006571808382864
0.9274827273832615    0.6433135365114581    -0.0041123519136544
0.4194983940763411    0.6306109819114738    0.4954731319825660
0.5694237588525626    0.6455231159148626    -0.0039221353799601
0.0685112048608989    0.8890570039950966    0.0021444304801911
0.9046265911142475    0.8970585436357903    0.4892338674598162
0.4281661656849901    0.9002914997595318    -0.0047349352367142
0.5814888869772864    0.8799284079261507    0.4972135287212757
0.2531099373148100    0.6430317428379569    -0.0029812850917371
0.7536651370188006    0.8858615045093591    0.0038692742069124
0.4717205169397075    0.0267202841896641    0.4956148000251905
0.0203067710605729    0.0520166050121333    0.5044089771220460
0.5364023534228024    0.2754809858651369    0.4943918074631705
0.5282081931585180    0.7764697602305272    0.4970668853599545
0.4689911460689994    0.5228592626888110    0.4949199257530785
0.0195298322297064    0.5662206028584501    0.5086000460447557

```

5. H₂V₂O₅

CONTCAR

1.0000000000000000

12.2461842050227450 -0.0070114737609187 -0.0063979993591103

-0.0040096335465414 7.4085338317862082 -0.0000164853384933

-0.0021531101989887 -0.0000351889147315 4.0213489964792215

V O H
8 20 8

Direct

0.1088869750475984	0.1528086005088387	0.0013156801539586
0.4012356687450179	0.1532382610831538	0.0036385109723512
0.9011295003187260	0.4041775829643247	-0.0045686593578314
0.6089015468001243	0.4014754161850526	-0.0002196978073868
0.1088869750475984	0.6528085855088410	0.0013156801539586
0.4012356687450179	0.6532382460831567	0.0036385109723512
0.9011295003187260	0.9041775829643246	-0.0045686593578314
0.6089015468001243	0.9014754161850523	-0.0002196978073868
0.0778770998441313	0.1403223081792670	0.5011634742880805
0.9199943787049375	0.1484385797079640	0.0071943478024080
0.4210702543793213	0.1367006326024385	0.4987176578709757
0.5734781580909765	0.1488133035643095	0.0010680932814849
0.0739106314448884	0.4001562887456511	-0.0009342181721453
0.9206323657203921	0.3870470355931715	0.5003130941067753
0.4202628296566235	0.3975336381076433	-0.0073068888043705
0.5781445500296967	0.3901342432290283	0.4994673518700276
0.2466077489395956	0.1529602164107028	0.0021079158244763
0.7467515613288764	0.4027449959174441	-0.0018167261746994
0.0778770998441313	0.6403222931792699	0.5011634742880805
0.9199943787049375	0.6484385647079663	0.0071943478024080
0.4210702543793213	0.6367006176024410	0.4987176578709757
0.5734781580909765	0.6488132885643124	0.0010680932814849
0.0739106314448884	0.9001562887456509	-0.0009342181721453
0.9206323657203921	0.8870470355931712	0.5003130941067753
0.4202628296566235	0.8975336381076434	-0.0073068888043705
0.5781445500296967	0.8901342432290281	0.4994673518700276
0.2466077489395956	0.6529602014107053	0.0021079158244763
0.7467515613288764	0.9027449959174443	-0.0018167261746994
0.0259340367042018	0.0350848033947011	0.5001853505093038
0.4768990476414287	0.0364546679709997	0.5002108311272137
0.9759712052979808	0.2862775486929251	0.4993974779970173
0.5257425253054897	0.2854918401424124	0.5000663375123653
0.0259340367042018	0.5350847963946969	0.5001853505093038
0.4768990476414287	0.5364546609709951	0.5002108311272137
0.9759712052979808	0.7862775486929245	0.4993974779970173
0.5257425253054897	0.7854918401424129	0.5000663375123653

6. $\text{Mg}_{0.25}\text{V}_2\text{O}_5$

CONTCAR

```

1.0000000000000000
 11.4622151976138316    0.0000000000000000    0.0000000000000000
   0.0000000000000000    7.1523068301985813    0.0000899853758472
   0.0000000000000000   -0.0000052546030792    4.6294273902446372
V      O      Mg
 8      20      1
Direct
0.1021426044811348  0.1311831272796716  0.8890415929320103
0.3978573885188681  0.1311831272796716  0.8890415929320103
0.8992797849725228  0.3750240230486920  0.1273819124421909
0.6007202150274772  0.3750240230486920  0.1273819124421909
0.1021403133409971  0.6188626344008907  0.8890291796867015
0.3978596796590059  0.6188626344008907  0.8890291796867015
0.9016862352329991  0.8750303584612311  0.1039082061732750
0.5983137647670009  0.8750303584612311  0.1039082061732750
0.1261233671502250  0.1711352645963513  0.5439995225222903
0.9323298528831031  0.1282666893592967  0.0005707015336080
0.3738766478497727  0.1711352645963513  0.5439995225222903
0.5676601931168975  0.1282666893592967  0.0005707015336080
0.0751722517650566  0.3750218321487029  0.0471046430719071
0.8942034252862505  0.3750005853866021  0.4744031228454991
0.4248277552349475  0.3750218321487029  0.0471046430719071
0.6057965747137495  0.3750005853866021  0.4744031228454991
0.2500000000000000  0.1347334137806581  0.0331894515187145
0.7500000000000000  0.3750377716630778  0.0121936613474608
0.1261288464170018  0.5789031031665461  0.5439867110706562
0.9323285958561357  0.6217754182234327  0.0005586259644906
0.3738711685829959  0.5789031031665461  0.5439867110706562
0.5676614501438649  0.6217754182234327  0.0005586259644906
0.0701121550674886  0.8750331606486192  0.9605684999367468
0.9049654747650312  0.8750257256392695  0.4518482105266657
0.4298878519325155  0.8750331606486192  0.9605684999367468
0.5950345252349688  0.8750257256392695  0.4518482105266657
0.2500000000000000  0.6153291956207531  0.0331804982038999
0.7500000000000000  0.8750295737790100  0.0049191514398590
0.2500000000000000  0.3750259674379397  0.3517153660779881

```

7. $\text{Mg}_{0.25}\text{H}_{0.5}\text{V}_2\text{O}_5$

CONTCAR

1.0000000000000000

11.6741397981165189	0.1702917246601370	0.0164954661659179
0.0773022504919605	7.2103463990489880	0.0848685618846499
0.0115479953257937	0.0396942182629270	4.4521253952314117

V	O	H	Mg
8	20	2	1

Direct

0.1047309814338129	0.1035605076215192	0.8947085989735133
0.4039159550718331	0.1474558232060593	0.8675576178402151
0.9024128424114319	0.3615845161150427	0.1296841382567960
0.6028508591684081	0.3799395565518766	0.1010186793117720
0.0980100430505193	0.5997583964187259	0.8730183990467073
0.3946435124442167	0.6437754060381528	-0.0228891930033745
0.9069895482287255	0.8621327973228852	0.1118549571224164
0.6076403234966983	0.8832174276142623	0.0919697199479024
0.1175376635704916	0.1307871273714898	0.5281040796888983
0.9380139097349024	0.1096325840133556	0.0077761035058389
0.3670748370338998	0.1968106111358097	0.5127630253616006
0.5739070348840605	0.1280895451972676	0.9688676351683644
0.0725388612448885	0.3517955205617824	0.0337132754918146
0.9025658267945394	0.3627628298418390	0.4921306015253398
0.4402265898093746	0.3850408344625328	0.0106076567557963
0.5882921433720172	0.4008345195007514	0.4914433485096967
0.2484558772649806	0.1358687124487936	0.0141411397661699
0.7553695066075584	0.3652322866309317	0.0347469449438846
0.1261793568153885	0.5620820268690971	0.5139919190880006
0.9347151277963744	0.6143916836986223	-0.0018193737174563
0.4171410419810967	0.6393095295347215	0.5251050404616069
0.5757082425165368	0.6377248075468919	0.0020572653435572
0.0793154747146236	0.8585326680305423	-0.0187195552234142
0.9088505771408496	0.8552128600086081	0.4740785245734532
0.4283146530261565	0.8892824563109293	-0.0100874930209141
0.5967526630343807	0.8848689500810473	0.4583014733414132
0.2525387560422760	0.5735411169048787	0.0308909970155848
0.7569165920400422	0.8759890370690840	0.0128432962929274
0.5160564017820796	0.4879256433674292	0.5200624444730930
0.4677807189809081	0.7475957098678573	0.5069609138386114
0.2221141015069147	0.3409645576572101	0.3348876853201945

8. Mg_{0.25}H₁V₂O₅

CONTCAR

1.0000000000000000

12.1666832373837188	0.0360194637730761	-0.0004097180790997
0.0159863688799579	7.3683205442142832	-0.0048148219932623
-0.0262893469711257	-0.0040321048622184	4.0579076550426363

V	O	H	Mg
8	20	4	1

Direct

0.0958456200927397	0.1077583682311470	0.8980103091030628
0.3927698841265679	0.1068038615721547	0.0048373202439278
0.9086260237381586	0.3617594807389548	0.1021188132526443
0.6124010074271503	0.3525555632438272	0.0070053815834035
0.1007048320209511	0.6227827688600869	0.9067847647835269
0.3960884290956898	0.6024671900896026	0.0053291421067025
0.8920668535665338	0.8605585560926811	0.0933212287584686
0.6014339225644905	0.8543821989443712	0.0141092654527795
0.1142441348500217	0.1305210916943549	0.4903310518253592
0.9409093849883297	0.0957117431751246	-0.0022084724433138
0.4100280575575099	0.1314199914962561	0.5066542095955355
0.5648721846131067	0.1022970280469427	0.0088586625848560
0.0688023996074096	0.3626226084470526	0.0145269599983424
0.9029224111710015	0.3620095496425518	0.5053871100762373
0.4335432077037545	0.3667036545193688	0.0060278475224104
0.5809703543842974	0.3651321276829809	0.5077652443381870
0.2519237843416750	0.1636422220375170	0.0156815871975383
0.7507062201852998	0.3551689123509659	0.0119808796949301
0.1103284201675775	0.5928002650134852	0.5000650666268447
0.9427897475166767	0.6248633625425034	-0.0003019115507049
0.4121173454255903	0.6212735411775002	0.5060833271015116
0.5727030451850667	0.6163294829491637	0.0086489016605117
0.1039143921518847	0.8566418466074395	-0.0245176097245800
0.9050291827773569	0.8610322417241891	0.4951690091770116
0.4146665438185217	0.8586736707432445	0.0055376790195621
0.5772741846112629	0.8680873572930848	0.5101636106287056
0.2458627106985100	0.5551121486894216	0.0222501769614104
0.7526071687738216	0.8616881013166362	0.0098009049610104
0.4677993795697266	0.7220033736309041	0.5082930998428017
0.5258337547238703	0.9730322679742565	0.5099306610557658
0.5324216186540912	0.4741148435196134	0.5068577727648134
0.4695459291281920	0.2265268502720242	0.5074114820211584
0.2003979527631626	0.3603136776805912	0.3610365987795622

9. $\text{Mg}_{0.25}\text{H}_{1.5}\text{V}_2\text{O}_5$

CONTCAR

1.0000000000000000			
12.3111438159647140	0.1020825330678561	0.0132462894560208	
0.0705426396814046	7.2709564340473163	0.0090095220551198	
0.0048581422001124	0.0121088899209088	4.0131921226459619	
V	O	H	Mg
8	20	6	1
Direct			
0.1082818838461392	0.1519144847926270	0.9983172654612034	
0.3903668760462367	0.1565329082181037	0.9931524345282412	
0.8939346404363562	0.3952990194974078	0.0670395120961871	
0.6039702745665991	0.4010101617222190	0.9867886923202605	
0.1010436071207081	0.6511672328539788	0.9916048121303334	
0.3904393402993662	0.6575610903209963	0.9918882547398482	
0.8961223616290894	0.9046652299988978	0.0780294204258567	
0.6056032007568177	0.8979698106121035	0.9940689566181220	
0.0932790448203136	0.1180949554030022	0.5025306133118974	
0.8926871846145161	0.1507056298744303	0.0078002317774448	
0.4190997204999007	0.1350495724487928	0.4930852271927719	
0.5967858361336340	0.1430296744760398	0.9917337869174432	
0.0563429793924684	0.3856216448214269	0.0050510412845597	
0.8877691621469808	0.4267717412600547	0.4890339185307653	
0.4329050657478604	0.3924348836655653	0.9923675272076480	
0.5875266776651529	0.3807313553934648	0.4890084868758748	
0.2497187525945037	0.1621412628177339	0.9964008482495643	
0.7468649426632439	0.4545148699382864	0.9755070283173097	
0.0871345032766939	0.6296153764100438	0.4948585217615360	
0.9291498006814649	0.6501936626508638	0.9748850839302108	
0.4126445688788039	0.6356421734223119	0.4916586546161170	
0.5618319561287421	0.6444501299019763	0.9893628172920970	
0.0556411856460315	0.9064746369203860	0.0062870728351498	
0.8872065331946430	0.8844333637392197	0.4942154121560876	
0.4353836925428212	0.9074800409688493	0.9937397299690076	
0.5986160535388549	0.8578551607088727	0.4924735127206716	
0.2468362300211879	0.6625458275750731	0.9916008266889378	
0.7503359585010188	0.8451616486608984	0.9844207081481713	
0.4520446352881677	0.0109391083727033	0.4938920845925949	
0.0637110212421348	0.9936514308334452	0.5076021053005064	
0.5416693504497303	0.2688631379571689	0.4894258078767351	
0.5422369677222250	0.7614088241634676	0.4935814389717308	
0.4621132467966405	0.5261364141521199	0.4914309015410367	
0.0206524201212517	0.5550553147726802	0.5022358979734847	
0.7894702609897166	0.6581282026748028	0.6122713636405877	

10. $\text{Mg}_{0.25}\text{H}_2\text{V}_2\text{O}_5$

CONTCAR

```

1.0000000000000000
  12.4625024904324384    0.0254813830695125    0.0080245900522564
    0.0077284771207168    7.4126290511295334   -0.0003200915876329
   -0.0013582153920789   -0.0002674126431777    4.0520348342339423
  V      O      H      Mg
    8      20      8      1
Direct
  0.1016288417386564   0.1588441605376255   0.0010865692869728
  0.3928913442645179   0.1648420919364742   0.0009861259470374
  0.8923914673135401   0.4092521798322708  -0.0008001028471751
  0.6012271215901026   0.4086578539082488   0.0004085712473256
  0.1023189135311013   0.6585336685959756   0.0006663451071601
  0.3997316562280346   0.6641232017558538   0.0011486670539737
  0.8924455040164200   0.9082457718635091   -0.0009229299376407
  0.6101997559145891   0.9117035659027327   0.0001160014722941
  0.0878804747565137   0.1326142702859742   0.4990092949626422
  0.9331395874354123   0.1379249695385378   -0.0005151736043561
  0.4126156933496852   0.1450231578090124   0.5006630911452322
  0.5595963256521413   0.1446767193887016   0.0003301635920815
  0.0629032412609712   0.4012550462468111   -0.0023299278818877
  0.9219588385361908   0.3963553152983646   0.4990003143368789
  0.4352463043894017   0.4082640301307869   0.0007382289317587
  0.5838587159363000   0.3881814097750511   0.5005176012418348
  0.2540614833533241   0.2004490748324171   -0.0000929324162879
  0.7536832416957578   0.4134049763178927   -0.0003031938336944
  0.1034634114521049   0.6035873538256579   0.4992979431804317
  0.9375659608311371   0.6679314477872124   -0.0002673360637713
  0.3982625001015277   0.6130557875843939   0.5009215202504119
  0.5635423352291894   0.6612561350305932   0.0008407901643551
  0.1051861875190788   0.8911949036057142   -0.0037820965364072
  0.9174805849986485   0.8886228686980351   0.4993139272955409
  0.4003103720467124   0.8985017731099479   0.0008141120078038
  0.5827331308019018   0.8908363352181530   0.5003622092178043
  0.2512047172649609   0.5813382046400347   0.0012869474914964
  0.7484342324502173   0.9020951436982406   -0.0003327465567117
  0.0367293864327166   0.0290285769657883   0.4995845142844146
  0.4559697894760384   0.0321175644148638   0.5006869299553204
  0.9663114057889571   0.2850678595147533   0.4990146778506721
  0.5312021022894431   0.2870309106155339   0.5005278523113713
  0.0399945717763030   0.5187161398644570   0.4999642309599067
  0.4601121141059252   0.5265358757049635   0.5009456269660127
  0.9419739493900595   0.7629003511918133   0.4991156892410634
  0.5656357395391483   0.7616450800999444   0.5000777924410923
  0.2529690235432522   0.4779162264736578   0.5019306237350326

```

4) The convergence test of the k -meshes of the V_2O_5

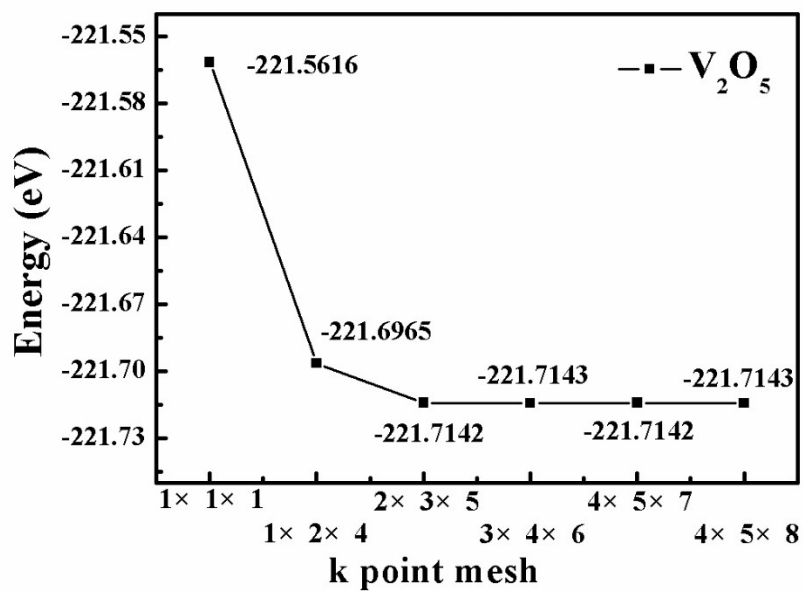


Fig. S2. Convergence test of the k -meshes.

5) Ab initio molecular dynamics calculations at 500 K were carried out for the V_2O_5 and $H_2V_2O_5$.

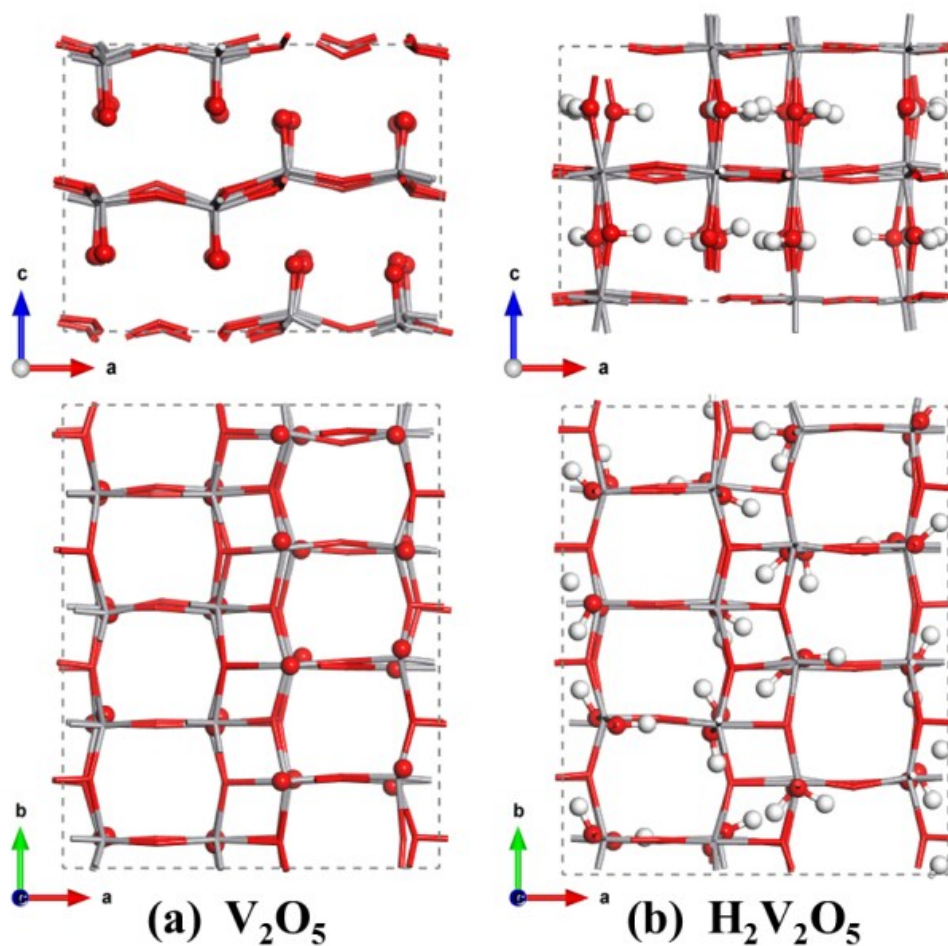


Fig. S3. Side (top) and top (bottom) views of the structures of V_2O_5 (a) and $H_2V_2O_5$ (b) at 500 K from ab initio molecule dynamics simulations.