

Supporting Information (SI)

Are MXenes Promising Anode Materials for Li Ion Batteries?
Computational Studies on Electronic Properties and Li Storage
Capability of Ti_3C_2 and $\text{Ti}_3\text{C}_2\text{X}_2$ (X= F, OH) Monolayer

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The optimized atomic coordinates of Ti_3C_2 , $\text{Ti}_3\text{C}_2\text{F}_2$, and $\text{Ti}_3\text{C}_2(\text{OH})_2$ unit cells and their 3×3 supercells with one adsorbed Li atom are given in the format of VASP input. Total energies are given in parenthesis.

(1) Unit cell of bare Ti_3C_2 monolayer (GGA/PBE level, spin-polarized free energy TOTEN: -43.539 eV)

```
1.0000000000000000
2.6883951985018508   -1.5514427239055619   0.0000111303329820
-0.0006087877982130   3.1039398992248510   -0.0000197140399680
-0.0000075989189900   0.0001016192400290   16.0000000145770898
2      3
Direct
C   0.6666666666666643   0.3333333333333357   0.5810337763008668
C   0.3333333333333357   0.6666666666666643   0.4189662236991332
Ti  0.0000000000000000   0.0000000000000000   0.5000000000000000
Ti  0.3333333333333357   0.6666666666666643   0.6450254278856442
Ti  0.6666666666666643   0.3333333333333357   0.3549745721143557
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(2) Unit cell of $\text{I-Ti}_3\text{C}_2\text{F}_2$ monolayer (GGA/PBE level, spin-non-polarized free energy TOTEN: -58.053 eV)

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1.0000000000000000
2.6645500583304198   -1.5316296137901599   0.0000087653755130
-0.0058448744167390   3.0733828470574100   -0.0000109911355460
-0.0000222353287620   0.0000643299215070   18.0000000166356990
2      2      3
Direct
C   0.6666666666666643   0.3333333333333357   0.5708079436322003
C   0.3333333333333357   0.6666666666666643   0.4291920563677997
```

F	0.0000000000000000	0.0000000000000000	0.2996291691980126
F	0.0000000000000000	0.0000000000000000	0.7003708308019874
Ti	0.0000000000000000	0.0000000000000000	0.5000000000000000
Ti	0.3333333333333357	0.6666666666666643	0.6312213134213988
Ti	0.6666666666666643	0.3333333333333357	0.3687786865786014

(3) Unit cell of II-Ti₃C₂F₂ monolayer (GGA/PBE level, spin-non-polarized free energy TOTEN: -57.262 eV)

1.0000000000000000			
2.6173519467205009	-1.5059897179922741	-0.0003572706553050	
-0.0044505903662610	3.0196881247412519	0.0004391860885860	
0.0009514957870860	-0.0026165333845640	17.9999998014423888	
2	2	3	
Direct			
C	0.6666666666666643	0.3333333333333357	0.5715154650554950
C	0.3333333333333357	0.6666666666666643	0.4284845349445049
F	0.3333333333333357	0.6666666666666643	0.2884952741186889
F	0.6666666666666643	0.3333333333333357	0.7115047258813114
Ti	0.0000000000000000	0.0000000000000000	0.5000000000000000
Ti	0.3333333333333357	0.6666666666666643	0.6372641223088149
Ti	0.6666666666666643	0.3333333333333357	0.3627358776911850

(4) Unit cell of III-Ti₃C₂F₂ monolayer (GGA/PBE level, spin-non-polarized free energy TOTEN: -57.658 eV)

1.0000000000000000			
2.6436511825105828	-1.5207677034592240	-0.0000265708682610	
-0.0048021267689730	3.0498529346229000	0.0000114383411790	
0.0001422093179410	-0.0000672843047300	18.0000000160767719	

2 2 3

Direct

C	0.6666666666666643	0.3333333333333357	0.5545860867378599
C	0.3333333333333357	0.6666666666666643	0.4119072785752403
F	0.0000000000000000	0.0000000000000000	0.2812227598944750
F	0.6666666666666643	0.3333333333333357	0.6927610420499061
Ti	0.6666666666666643	0.3333333333333357	0.3510102707977899
Ti	0.3333333333333357	0.6666666666666643	0.6192006284230087
Ti	0.0000000000000000	0.0000000000000000	0.4845947911438409

(5) Unit cell of I-Ti₃C₂(OH)₂ monolayer (GGA/PBE level, spin-non-polarized free energy TOTEN: -69.682 eV)

1.0000000000000000

2.6716879598820169	-1.5425007115138700	-0.0000008215851960
0.0000000000000000	3.0849999999998912	-0.0000008215851960
0.0000000000000000	0.0000000000000000	18.0000000000000000

2 2 2 3

Direct

H	0.9197470194696413	0.0661683374794537	0.2280961832876358
H	0.8935752062333908	0.0946651800286864	0.7408392120372126
C	0.5741558985279968	0.4112731056588713	0.5552351549801399
C	0.2425217000050252	0.7426725853414372	0.4135645140970763
O	0.9110376382481189	0.0743777702487720	0.2821101560435774
O	0.9072408560339147	0.0842667884022712	0.6868939161192414
Ti	0.9076924788192142	0.0771341497096362	0.4846075000475426
Ti	0.2406788242654608	0.7473840554574422	0.6159620360539023
Ti	0.5765298514180683	0.4090738149373641	0.3530977261068649

(6) Unit cell of II-Ti₃C₂(OH)₂ monolayer (GGA/PBE level, spin-non-polarized free energy TOTEN: -69.171 eV)

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1.0000000000000000
2.6348753015621811  -1.5157035726880981  -0.0003443358791780
-0.0047998249921640   3.0397207230236378   0.0004258048272630
0.0009026779718310  -0.0025200190484420   17.9999998344919021
 2   2   2   3
Direct
H  0.6666666666666643  0.3333333333333357  0.7632881111465522
H  0.3333333333333357  0.6666666666666643  0.2367118888534478
C  0.6666666666666643  0.3333333333333357  0.5708320020152471
C  0.3333333333333357  0.6666666666666643  0.4291679979847529
O  0.3333333333333357  0.6666666666666643  0.2908090153725885
O  0.6666666666666643  0.3333333333333357  0.7091909846274115
Ti 0.3333333333333357  0.6666666666666643  0.6352991925495399
Ti 0.6666666666666643  0.3333333333333357  0.3647008074504602
Ti 0.0000000000000000  0.0000000000000000  0.5000000000000000

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(7) Unit cell of III-Ti₃C₂(OH)₂ monolayer (GGA/PBE level, spin-non-polarized free energy TOTEN: -69.433 eV)

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1.0000000000000000
2.6524811470992171  -1.5277643834989520  -0.0008676377648000
-0.0031576329436650   3.0609981781121709   0.0010876342054650
0.0022053833319220  -0.0063934865121980   17.9999987629624023
 2   2   2   3
Direct
H  0.6608847886999527  0.3343166204930979  0.7619144150613389
H  0.0120521173441955  0.9768008560451986  0.2414738718356424

```

C	0.6667362647940087	0.3318409971621691	0.5700810507672537
C	0.3362376194353187	0.6592340127379425	0.4275111272446796
O	0.0034273928971365	0.9917341102692322	0.2955991308507617
O	0.6638318262845543	0.3330395304710471	0.7076399969427122
Ti	0.0007383964344272	0.9966772131977618	0.4996665231395062
Ti	0.3327198238431663	0.6653107346351356	0.6343800140132918
Ti	0.6702923388634225	0.3252812427724090	0.3662957348395638

(8) 3×3 supercell of Ti₃C₂ monolayer with one adsorbed Li (GGA/PBE+D2 level, spin-polarized free energy TOTEN: -405.679 eV)

1.0000000000000000			
8.0642720816605102	-4.6559110889292299	-0.0000012399438390	
0.0000000000000000	9.3118200302123206	-0.0000012399438390	
0.0000000000000000	0.0000000000000000	16.0000000000000000	
1	18	27	
Direct			
Li	0.4445984243501911	0.5554985847425311	0.2011916278704516
C	0.2216008472466841	0.1106026017426772	0.5816444177825717
C	0.1107330830634561	0.2218096017641137	0.4181650308027762
C	0.5561011133280999	0.1115951860392842	0.5811518989558924
C	0.4448761553779553	0.2225880172515673	0.4185091541798160
C	0.8891153426069203	0.1109201239637076	0.5812720451389152
C	0.7774982324735386	0.2224732077214113	0.4185417333169718
C	0.2221150824219131	0.4446487480086014	0.5812597915053145
C	0.1117370596913024	0.5560895940330923	0.4184001107600929
C	0.5559674476361672	0.4440300579607036	0.5816045206712889
C	0.4450137891919570	0.5550253673941248	0.4221223476010805
C	0.8884110375467128	0.4438839267180355	0.5811527267388190
C	0.7773884005262487	0.5551154084355417	0.4185096246576068

C	0.2222511503191033	0.7777298647330360	0.5810403921404987
C	0.1108141351691536	0.8891755259629952	0.4172788781723930
C	0.5553595799624962	0.7778596084621903	0.5812726525333670
C	0.4438773586472908	0.8882638401050850	0.4184030862737411
C	0.8893780869283008	0.7783492874908026	0.5816404516637592
C	0.7782683856560811	0.8893135817084923	0.4181836701589051
Ti	0.0000852317273948	0.0000133798081184	0.4998566437536385
Ti	0.1111620747146371	0.2223783924619597	0.6456328415483440
Ti	0.2230529407412598	0.1128783821960810	0.3534152769829733
Ti	0.3327066510454246	0.9997604222135172	0.4998260456714994
Ti	0.4441593166935133	0.2217627172518694	0.6458767048204985
Ti	0.5550491256962512	0.1109929758542340	0.3541274744281188
Ti	0.6663771397144621	0.9996808150877398	0.4998743431099709
Ti	0.7780308895533370	0.2219646786510930	0.6455598985571925
Ti	0.8887377511061959	0.1112451626767382	0.3541612851360799
Ti	0.0003207026581826	0.3336308335780940	0.4998524253953427
Ti	0.1110399636119499	0.5557694999117810	0.6456657236642159
Ti	0.2259610812593486	0.4461747435834857	0.3546598330868919
Ti	0.3328749761375247	0.3324432829207120	0.5004161560904862
Ti	0.4443813741670422	0.5556239884846765	0.6458543356582219
Ti	0.5538155870476132	0.4461905493050067	0.3547098854550630
Ti	0.6667057150077047	0.3332934406713421	0.4999992171157017
Ti	0.7782288558853219	0.5558428602026393	0.6458951708028692
Ti	0.8889926148279230	0.4449421277782916	0.3541635751303893
Ti	0.0002299669170344	0.6672649514693156	0.4998022963372437
Ti	0.1113161953516696	0.8886632074846248	0.6459384936766334
Ti	0.2226359781454929	0.7773499436482861	0.3534655050731747
Ti	0.3332196014056860	0.6667739850244697	0.5002934178024713
Ti	0.4442285190606068	0.8889426627587735	0.6456598824017129
Ti	0.5538440824160534	0.7741117485724407	0.3546693863944981

Ti	0.6675380107434535	0.6671228054489191	0.5004079192434359
Ti	0.7776639005940004	0.8888303652610927	0.6456580950704731
Ti	0.8871104078164408	0.7769097393545092	0.3534103284010681

(9) 3×3 supercell of I-Ti₃C₂F₂ monolayer with one adsorbed Li (GGA/PBE+D2 level, spin-polarized free energy TOTEN: -538.948 eV)

1.0000000000000000			
7.9849008515769304	-4.6100860737826803	-0.0000012277399020	
0.0000000000000000	9.2201700210570596	-0.0000012277399020	
0.0000000000000000	0.0000000000000000	18.0000000000000000	
1	18	18	27
Direct			
Li	0.4447286834412253	0.5552716186068251	0.2363342326141503
C	0.2224194334953105	0.1112515248555777	0.5714108471222723
C	0.1111865745812247	0.2220389061409274	0.4281334114676455
C	0.5553065065784251	0.1111667202318487	0.5712998384494627
C	0.4443975460207118	0.2221868491364961	0.4281921705529132
C	0.8887898893080856	0.1112101063514733	0.5710091183696042
C	0.7775245681347432	0.2224754351399542	0.4281435747133068
C	0.2223024945941402	0.4448499171129694	0.5715458787745544
C	0.1108348935097523	0.5561519347472716	0.4283042260620032
C	0.5551792238416382	0.4448207720494661	0.5713889392964695
C	0.4442793340444174	0.5557206681863472	0.4285200002970071
C	0.8888332757861833	0.4446934894219182	0.5712998384299645
C	0.7778131544321357	0.5556024577899621	0.4281921704530034
C	0.2223238277803618	0.7776761681273408	0.5716510599804541
C	0.1112467543857247	0.8887532494367121	0.4289838834263928
C	0.5551500786039395	0.7776975011679713	0.5715458788700066
C	0.4438480672821141	0.8891651068404280	0.4283042242771711

C	0.8887484708415747	0.7775805621720407	0.5714108470279086
C	0.7779610959040499	0.8888134258381762	0.4281334094830745
F	0.0023165633083230	0.9976834377710766	0.2977869381797724
F	0.9998590290307280	0.0001409693908029	0.7005940555826798
F	0.3303592238016949	0.9981058970021525	0.2976078036606313
F	0.3317723385239677	0.0001453635430747	0.7013783407271587
F	0.6665239836446374	0.9966573078845917	0.2976684710584531
F	0.6683180006264244	0.0001173952768204	0.7012361160808039
F	0.0033426920613353	0.3334760177732667	0.2976684713076228
F	0.9998826029006314	0.3316819975698903	0.7012361161124809
F	0.3413853136691696	0.3501588806072342	0.2898976553623718
F	0.3316478303255904	0.3319708503606542	0.7012966368074843
F	0.6656193948765726	0.3343806078677189	0.2976160093183338
F	0.6666774498906707	0.3333225479913068	0.7015065291146708
F	0.0018941049752875	0.6696407788138795	0.2976078035477435
F	0.9998546344952343	0.6682276594182361	0.7013783406291128
F	0.3430162623483530	0.6569837381466160	0.2900089259264358
F	0.3332460510690801	0.6667539469324435	0.7015526408681044
F	0.6498410935181985	0.6586146733336302	0.2898976517133531
F	0.6680291478136822	0.6683521677016252	0.7012966366502442
Ti	0.9998887676435536	0.0001112313319690	0.5000299709246599
Ti	0.1110261039131102	0.2222459984809977	0.6312052443050414
Ti	0.2205733589656114	0.1080322724952092	0.3688082581066930
Ti	0.3341992033969059	0.0003429207961400	0.5001169374841213
Ti	0.4442303991985816	0.2222148066507169	0.6316044760657469
Ti	0.5553520561956875	0.1109745998561210	0.3683363702100741
Ti	0.6662345067490595	0.0004985564777030	0.5000147973897501
Ti	0.7778494437613429	0.2221505444411654	0.6315043652218830
Ti	0.8887792643401911	0.1112207450593465	0.3685954665566806
Ti	0.9995014408481012	0.3337654916884027	0.5000147989970042

Ti	0.1107335711810200	0.5554513779989946	0.6317512109839231
Ti	0.2197740750401826	0.4433073489020635	0.3701702682890461
Ti	0.3334878742236886	0.3335755590024699	0.4999184120725142
Ti	0.4444661963965650	0.5555337924402368	0.6316749187453596
Ti	0.5566126234963459	0.4433873928947740	0.3700907242918217
Ti	0.6667384866265430	0.3332615130841624	0.5000162574163670
Ti	0.7777851817452874	0.5557695894084795	0.6316044762741367
Ti	0.8890254104959604	0.4446479555310724	0.3683363703860339
Ti	0.9996570785080835	0.6658007957827472	0.5001169376201373
Ti	0.1110655222644255	0.8889344661549579	0.6313965697048108
Ti	0.2205639563364051	0.7794360563882192	0.3686276160992572
Ti	0.3330615334817649	0.6669384643988948	0.5001276563356717
Ti	0.4445486105993555	0.8892664174365699	0.6317512110941904
Ti	0.5566926590380435	0.7802259246494931	0.3701702539512370
Ti	0.6664244405755311	0.6665121243255924	0.4999184103080208
Ti	0.7777539895746073	0.8889738842658401	0.6312052445198552
Ti	0.8919677344961214	0.7794266512745617	0.3688082576729536

(10) 3×3 supercell of I-Ti₃C₂(OH)₂ monolayer with one adsorbed Li (GGA/PBE+D2 level, spin-polarized free energy TOTEN: -644.126 eV)

1.0000000000000000			
8.0150633625644492	-4.6275032590334000	-0.0000036971334290	
0.0000000000000000	9.2550001144401808	-0.0000036971334290	
0.0000000000000000	0.0000000000000000	18.0000000000000000	
18	1	18	18
Direct			
H	0.3048437940688842	0.0257370610540339	0.2287428116261877
H	0.3026759776029413	0.0311093458969664	0.7392767601865783
H	0.6382972531522487	0.0258906456484727	0.2296338584781891

H	0.6351687392766935	0.0285384950513625	0.7390883615384416
H	0.9709559242261705	0.0247477290233664	0.2296966054132875
H	0.9684557145044367	0.0292797657019519	0.7390856599701751
H	0.3058969978272194	0.3580574864797970	0.2291763172358764
H	0.2470580328208790	0.3367561410311584	0.7396158216256568
H	0.6364787666202593	0.3575433856421480	0.2290452377726396
H	0.6633484571436861	0.3318864562516601	0.7397479736522464
H	0.9704949364753470	0.3577780798131462	0.2296548354470320
H	0.9683179417893513	0.3608998210856338	0.7390475136231971
H	0.3042248123315185	0.6907332346531541	0.2291527580670028
H	0.3018434240998998	0.6913628447264034	0.7392414298884538
H	0.6374710632195943	0.6901202534939114	0.2295356854600055
H	0.6588535879276807	0.7490486940162763	0.7396533225520233
H	0.9698616997506281	0.6902926709180958	0.2291298218514449
H	0.9647509984865154	0.6920478990561832	0.7389627026967627
Li	0.5251007005467770	0.4707232835334740	0.7324372728138450
C	0.1911855475873532	0.1368964444114230	0.5545609770462692
C	0.0810784307858906	0.2490561694288009	0.4138904605558260
C	0.5246755828400356	0.1369737391451944	0.5545024895531406
C	0.4140956871170708	0.2485156043805365	0.4140806671088219
C	0.8582225932238760	0.1371830001332850	0.5541120876786699
C	0.7470223039186012	0.2490517437492135	0.4137738610103214
C	0.1910554093916939	0.4704249099378403	0.5545027339940455
C	0.0807233811436963	0.5816659022500053	0.4134322421168495
C	0.5242186418616245	0.4701369769344277	0.5587824038251001
C	0.4140790518304293	0.5818547774437096	0.4139914191125775
C	0.8579093266822869	0.4707847724916462	0.5544702716617850
C	0.7473251152980697	0.5818264619624540	0.4139389759088004
C	0.1915704751722632	0.8037538197133176	0.5543712341109504
C	0.0808662706957523	0.9153896686676185	0.4129514543744596

C	0.5246064819194539	0.8035941407978990	0.5551916561288631
C	0.4142695987778750	0.9153998019964321	0.4129509431452854
C	0.8576243653694191	0.8036940611826959	0.5548386552517327
C	0.7471983015564021	0.9147247371775282	0.4137650289866706
O	0.3034249162735036	0.0269857524409328	0.2827302796837536
O	0.3019044839401317	0.0260556493384367	0.6851637958544006
O	0.6370089268600291	0.0269311497042319	0.2836110855828143
O	0.6364820034254628	0.0270224438997340	0.6848833386374364
O	0.9698742779634013	0.0268341314722982	0.2836966962608294
O	0.9694254162002712	0.0274851656813491	0.6848616626118399
O	0.3039907035617646	0.3597122042950453	0.2831275373412658
O	0.3065197203234631	0.3620764816773601	0.6920847860335589
O	0.6358049308236182	0.3598114270788262	0.2829868971845338
O	0.6338179211554972	0.3607391059090510	0.6920079009964627
O	0.9697446504629736	0.3595502337258591	0.2835449531542126
O	0.9690422104769885	0.3589466443639001	0.6848545012994909
O	0.3028012608633168	0.6921192715637160	0.2831478934088827
O	0.3014395430902385	0.6924896765739785	0.6850808569477649
O	0.6360387082063991	0.6918827311115331	0.2835394327440492
O	0.6335456855796547	0.6896129105449916	0.6921705390594940
O	0.9693338685093451	0.6921578913526548	0.2831380363504080
O	0.9696245070576670	0.6927579024122068	0.6849055179987228
Ti	0.3023716289698858	0.0254913323055865	0.4837738438927244
Ti	0.0789773435540403	0.2475639413789047	0.6140338892866642
Ti	0.1925289271170487	0.1382607754842485	0.3532365560188626
Ti	0.6355128982087659	0.0257696583888063	0.4838288653224382
Ti	0.4105054857270541	0.2419971171185863	0.6149795760642356
Ti	0.5251342779489937	0.1380780814738089	0.3531758057244861
Ti	0.9695438416960310	0.0256137391631887	0.4838326529935600
Ti	0.7475031151883977	0.2475962066820619	0.6139708472385407

Ti	0.8589115382329009	0.1382435755488585	0.3537238913202711
Ti	0.3034954215336823	0.3599475201806418	0.4848482291286762
Ti	0.0802594786215678	0.5813829617255031	0.6148659780368275
Ti	0.1920977457897921	0.4710279288353068	0.3533858509683054
Ti	0.6353744267305524	0.3599528046804739	0.4846934860105891
Ti	0.4100947807664972	0.5839285340628455	0.6152973690004740
Ti	0.5248709778003893	0.4702779250870028	0.3535251780214683
Ti	0.9695562252135962	0.3601266982051720	0.4838687207268613
Ti	0.7523969144605538	0.5839530938376556	0.6150898282803858
Ti	0.8585370368138477	0.4710124163943611	0.3533306372826686
Ti	0.3028684590373940	0.6934967519849703	0.4840093521760895
Ti	0.0803026438118378	0.9149803525429157	0.6149438179649132
Ti	0.1919055618584910	0.8040403718417973	0.3527121044631203
Ti	0.6353629371873157	0.6917497037698725	0.4848350614800203
Ti	0.4134284232760642	0.9150599349340802	0.6150020077413286
Ti	0.5250339316101116	0.8035416281038463	0.3533573008920260
Ti	0.9699456209251550	0.6933677297649301	0.4839103153523930
Ti	0.7478712980312504	0.9169865438137386	0.6141653319787286
Ti	0.8582608172095251	0.8035239158822159	0.3533617425264795