

Supplementary Information for "First-principles insights into the Janus MoPC monolayer as a promising anode for sodium-ion batteries"

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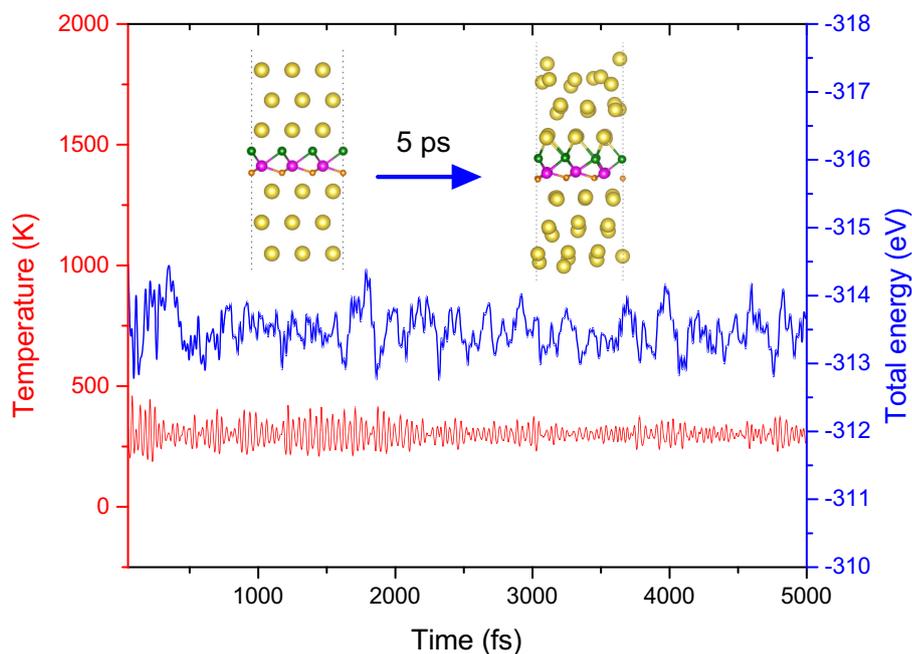


FIG. S1: Ab initio molecular dynamics (AIMD) simulation results for the Na₆MoPC configuration at 300 K over 5 ps. The temperature fluctuates around 300 K and the total energy exhibits only small oscillations without noticeable drift, indicating dynamical stability within the simulated time window.

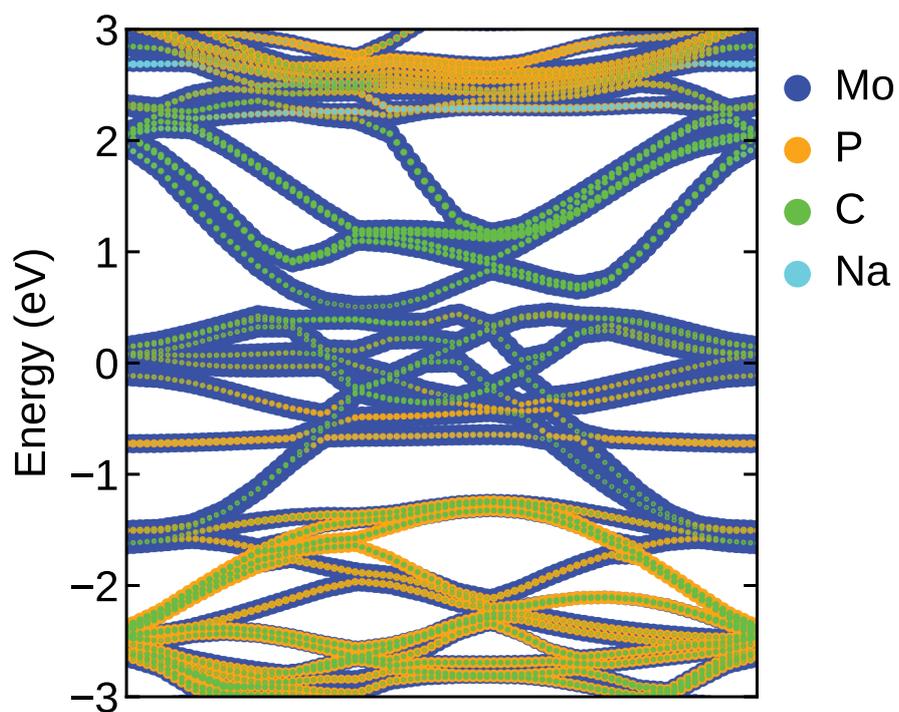


FIG. S2: Atom-projected electronic band structure of the most stable single-Na-adsorbed configuration on a 3×3 MoPC supercell calculated using the HSE06 hybrid functional (single-point on the PBE-relaxed geometry). The Fermi level is set to 0 eV, and bands are observed to cross the Fermi level without opening a band gap.

Optimized structure of MoPC Monolayer

```

C Mo P
1.0000000000000000
 3.4309043455809851 -0.0000012739726676 0.0000004394529628
-1.7154532760831864 2.9712496842412888 -0.0000004394529628
 0.0000020854992214 -0.0000012040635369 16.5679325707707576
  C Mo P
  1 1 1
Selective dynamics
Direct
 0.0000003600948803 -0.0000003600948803 0.4551960813479345
 0.6666665090693868 0.3333334909306132 0.4750241511733270
 0.0000001308357297 -0.0000001308357297 0.5697797674787385

 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.00000000E+00 0.00000000E+00 0.00000000E+00
 0.00000000E+00 0.00000000E+00 0.00000000E+00

```

Optimized structure of the 3x3 MoPC supercell

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Mo9 P9 C9
1.0000000000000000
10.2927129999999991 -0.0000040000000000 0.0000010000000000
-5.1463599999999996 8.9137489999999993 -0.0000010000000000
 0.0000020000000000 -0.0000010000000000 16.8984169999999985
  C Mo P
  9 9 9
Selective dynamics
Direct
 0.0000002139200886 -0.0000002277934878 0.4562237287741340
-0.0000187418267994 0.3334229735287437 0.4559428830618810
-0.0000190936092889 0.6665580209044750 0.4559428138900239
 0.3334419709746959 0.0000190860364611 0.4559428327840584
 0.3334421008764109 0.3334231663438326 0.4559429343068491
 0.3333330206927324 0.6666669748321219 0.4560347492802957
 0.6665770355743239 0.0000187422292593 0.4559428931364568
 0.6666668196157369 0.3333331961992114 0.4560437578464378
 0.6665768419822943 0.6665578983856778 0.4559429317571581
 0.222235792197724 0.1111117738449657 0.4755356419678733
 0.2222086372117372 0.4444168251886560 0.4755162293633751
 0.2222082502580931 0.7777917855881068 0.4755162159964310
 0.5555531586063389 0.1111059846510015 0.4755843461885484
 0.5555532915497555 0.4444467215181910 0.4755843977309577
 0.5555831868954858 0.7777913787575412 0.4755162285946224
 0.8888884752163060 0.1111115065325989 0.4755355654167126
 0.8888940007748938 0.4444468342339066 0.4755843419526416
 0.8888882139699513 0.7777764261787325 0.4755356362894671
-0.0000000094549946 0.000000008865321 0.5686737564338262
 0.0000150155503823 0.3330952565570704 0.5684186224747161
 0.0000148474891169 0.6669196574281639 0.5684186180388637
 0.3330803307647466 -0.0000148552749426 0.5684186129109601
 0.3330804178673290 0.3330953254457631 0.5684186580352693
 0.3333332338761955 0.6666667562234114 0.5684603660873445
 0.6669047493461312 -0.0000150189891926 0.5684186217465922

```


Selective dynamics

Direct

-0.0000639157938703	-0.0000099257783124	0.4668926031762101
0.9999035685604366	0.3337115537354706	0.4671925901250525
-0.0000697421171045	0.6663523454172293	0.4671832418457759
0.3335061864694550	-0.0000767806278634	0.4671931326764358
0.3334980718984769	0.3337296415667914	0.4671982352522064
0.3332611831276607	0.6666918380709528	0.4671605283923078
0.6662434081372155	-0.0000053626802408	0.4671794630799014
0.6665388560666147	0.3333430229203699	0.4672758125896249
0.6661856646052112	0.6663877154448630	0.4671984067794461
0.2219060121805456	0.1110114854935352	0.4873902572243304
0.2221247245382860	0.4445031902891380	0.4874581537464087
0.2221294118608273	0.7777544608026636	0.4874558611115545
0.5553986959604073	0.4444943552723805	0.4874904590148859
0.5554023779445795	0.1110052115907871	0.4875048290768139
0.8888990294144210	0.1110192134628297	0.4873932752132482
0.8888721179358553	0.4445105072661706	0.4875051714555647
0.8889053155508115	0.7780142140704317	0.4873852002712333
0.5554519581904627	0.7778094284757663	0.4874626387002920
0.5557349999999985	0.7778840000000002	0.7727130000000031
0.5556020000000004	0.4443580000000011	0.5940680000000000
0.2222360000000023	0.4444450000000018	0.5940930000000009
0.2222200000000001	0.7777969999999996	0.5941180000000017
0.2219660000000019	0.1109920000000031	0.5941299999999998
0.4443407220268061	0.5556363805959441	0.4120900477746625
0.4443537064871368	0.8887806582757450	0.4120874232080177
0.8887690000000035	0.1112049999999982	0.5941919999999996
0.2222774525272257	0.1111500014496331	0.3197343290359880
0.8889399999999981	0.1111459999999980	0.7726800000000011
0.5556679999999972	0.4444220000000030	0.7727229999999992
0.5556630000000027	0.1112770000000012	0.7727199999999996
0.7778863962462352	0.5556951168281236	0.2270762723385496
0.8889429999999976	0.7778259999999975	0.7726749999999996
0.2222080000000020	0.4443550000000016	0.7727190000000022
0.2222030000000004	0.7778890000000018	0.7727140000000006
0.2222620000000006	0.1111450000000005	0.7726789999999966
0.4444434193132140	0.5556516159772626	0.2270186209790651
0.4444482195266198	0.8887984838525956	0.2270218829521364
0.4443923153441787	0.2222034982861211	0.2270697005045297
0.2222610771499902	0.7778423637543926	0.3196877783797592
0.7778540488829453	0.8889348673242402	0.2270370932671625
0.7778844129515201	0.2222086081743909	0.2270875546731245
0.1111594121473085	0.8889261143780605	0.2270352364333298
0.8888159999999985	0.4444289999999995	0.7727160000000026
0.8888170000000031	0.4444620000000015	0.5940569999999994
0.4443491086284295	0.222218302841139	0.4121328796087966
0.5556389999999993	0.7778229999999979	0.5940950000000029
0.5556470243084055	0.7778341944026070	0.3196900922415434
0.5556455262568458	0.4444572551530395	0.3197356167322564
0.1111679999999993	0.2222480000000004	0.6830929999999995
0.1111689999999967	0.8889240000000029	0.6830980000000011
0.8889449949963569	0.1111448140385091	0.3197439642350815
0.7778380000000027	0.2222539999999995	0.6830610000000021
0.5556351342360719	0.1112170610656185	0.3197389241338709
0.7778429999999972	0.8889220000000009	0.6831000000000031

