

Supporting data for: Modelling interfacial ionic transport in $\text{Li}_2\text{VO}_2\text{F}$ cathodes during battery operation

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The fortran code used in the kinetic Monte-Carlo simulations can be found here:

https://github.com/jollactic/MC_Hopper

A List of optimised DFT structures in POSCAR-format are provided below:

```
Li2V02F_BULK
1.0000000000000000
  8.8753919874421268   -0.0125971117202002   -0.0089344167860407
  5.9735692410598942   10.2648587893524734    0.0003625160092420
  5.9735692410598924    3.3944068954591877    9.6873798276326326
  V      Li      O      F
  16     32     32     16
Direct
0.0785580956272842   0.0621661316681020   0.0621661316681020
0.0785467059393940   0.0621639909389509   0.3121743931036770
0.0785349111011207   0.0621735275170968   0.5621756483164009
0.0785476578706097   0.0621730853833670   0.8121649966160408
0.0785467059393940   0.3121743931036770   0.0621639909389509
0.0785575064714669   0.3121670472959662   0.3121670472959662
0.0785456616412455   0.3121647237500960   0.5621753435545583
0.0785354183342581   0.3121750050731728   0.8121744846094598
0.0785349111011207   0.5621756483164009   0.0621735275170968
0.0785456616412455   0.5621753435545583   0.3121647237500960
0.0785555867496897   0.5621680424673628   0.5621680424673628
0.0785457974275550   0.5621655547639769   0.8121733834617016
0.0785476578706097   0.8121649966160408   0.0621730853833670
0.0785354183342581   0.8121744846094598   0.3121750050731728
0.0785457974275550   0.8121733834617016   0.5621655547639769
0.0785551172139346   0.8121668376770653   0.8121668376770653
```

0.4189648103072292	0.0604058713733996	0.0604058713733996
0.7381144862266361	0.0639394553331634	0.0639394553331634
0.4190475529234335	0.0603775237314666	0.3103736252442775
0.7380673848145690	0.0639599777566460	0.3139613884368704
0.4191414267960272	0.0603363014793725	0.5603367019108142
0.7379879049954249	0.0639880543004832	0.5639894207368655
0.4190506915080650	0.0603713310991249	0.8103766790504463
0.7380706337633016	0.0639612329503026	0.8139581752353583
0.4190475529234335	0.3103736252442775	0.0603775237314666
0.7380673848145690	0.3139613884368704	0.0639599777566460
0.4189691591852395	0.3104050312025722	0.3104050312025722
0.7381205788413071	0.3139399258288413	0.3139399258288413
0.4190441821539870	0.3103777553587976	0.5603736259933612
0.7380634041228752	0.3139600591200432	0.5639623840993632
0.4191421256007593	0.3103348065944508	0.8103355868727109
0.7379864820819358	0.3139901041148922	0.8139892892097682
0.4191414267960272	0.5603367019108142	0.0603363014793725
0.7379879049954249	0.5639894207368655	0.0639880543004832
0.4190441821539870	0.5603736259933612	0.3103777553587976
0.7380634041228752	0.5639623840993632	0.3139600591200432
0.4189700851730433	0.5604056874202309	0.5604056874202309
0.7381240217030480	0.5639381897283839	0.5639381897283839
0.4190462028250849	0.5603766208215019	0.8103732406467526
0.7380648478367614	0.5639605923863863	0.8139619299531831
0.4190506915080650	0.8103766790504463	0.0603713310991249
0.7380706337633016	0.8139581752353583	0.0639612329503026
0.4191421256007593	0.8103355868727109	0.3103348065944508
0.7379864820819358	0.8139892892097682	0.3139901041148922
0.4190462028250849	0.8103732406467526	0.5603766208215019
0.7380648478367614	0.8139619299531831	0.5639605923863863
0.4189646427506515	0.8104066110359235	0.8104066110359235
0.7381197958916699	0.8139385310901948	0.8139385310901948
0.9210945440146037	0.1848594201274139	0.1848594201274139
0.2360423537969503	0.1894725844174942	0.1894725844174942
0.9210412252287450	0.1848647598853647	0.4348834615647301
0.2360586399071886	0.1894477617039317	0.4394807330288876
0.9209913700580589	0.1848884757867894	0.6848881111409355
0.2360768560952873	0.1894575970366881	0.6894578596706749
0.9210412159328834	0.1848820363772733	0.9348650518917112
0.2360552727658781	0.1894803288967062	0.9394492809100901
0.9210412252287450	0.4348834615647301	0.1848647598853647
0.2360586399071886	0.4394807330288876	0.1894477617039317
0.9210924650064207	0.4348589681021345	0.4348589681021345
0.2360394868938037	0.4394722193607745	0.4394722193607745
0.9210414541243471	0.4348641353158140	0.6848839035669066
0.2360561940538301	0.4394493252985745	0.6894808069270070
0.9209915774917052	0.4348865454631207	0.9348877815512709
0.2360760081484036	0.4394569092676445	0.9394571798182734
0.9209913700580589	0.6848881111409355	0.1848884757867894
0.2360768560952873	0.6894578596706749	0.1894575970366881
0.9210414541243471	0.6848839035669066	0.4348641353158140

0.2360561940538301	0.6894808069270070	0.4394493252985745
0.9210918515442063	0.6848601537216946	0.6848601537216946
0.2360410463532627	0.6894718564371835	0.6894718564371835
0.9210405708051217	0.6848633675494141	0.9348838269939542
0.2360533799497207	0.6894490824611107	0.9394817782001168
0.9210412159328834	0.9348650518917112	0.1848820363772733
0.2360552727658781	0.9394492809100901	0.1894803288967062
0.9209915774917052	0.9348877815512709	0.4348865454631207
0.2360760081484036	0.9394571798182734	0.4394569092676445
0.9210405708051217	0.9348838269939542	0.6848633675494141
0.2360533799497207	0.9394817782001168	0.6894490824611107
0.9210936480945704	0.9348598790790694	0.9348598790790694
0.2360459837991668	0.9394705395224513	0.9394705395224513
0.5785708542573951	0.1871661084579769	0.1871661084579769
0.5785646346964030	0.1871879173508679	0.4371428271115104
0.5785558804378498	0.1871660807099125	0.6871677650299768
0.5785621329233654	0.1871425333405082	0.9371884375748276
0.5785646346964030	0.4371428271115104	0.1871879173508679
0.5785631451440232	0.4371676844867777	0.4371676844867777
0.5785636491567556	0.4371878779860118	0.6871433275771326
0.5785558318598980	0.4371677843169348	0.9371645393908747
0.5785558804378498	0.6871677650299768	0.1871660807099125
0.5785636491567556	0.6871433275771326	0.4371878779860118
0.5785637755471448	0.6871678891608758	0.6871678891608758
0.5785629274610972	0.6871864626995308	0.9371435191330055
0.5785621329233654	0.9371884375748276	0.1871425333405082
0.5785558318598980	0.9371645393908747	0.4371677843169348
0.5785629274610972	0.9371435191330055	0.6871864626995308
0.5785713337413680	0.9371656182852465	0.9371656182852465

LiF_BULK

1.0000000000000000		
4.0573833270957111	-0.0000000000000000	0.0000000000000000
-0.0000000000000000	4.0573833270957111	0.0000000000000000
-0.0000000000000000	0.0000000000000000	4.0573833270957111

Li F
4 4

Direct

0.0000000000000000	-0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	-0.0000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.5000000000000000
0.5000000000000000	-0.0000000000000000	-0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.5000000000000000

LiF_100_SURFACE

1.0000000000000000		
4.0573829999999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	4.0573829999999997	0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

Li F

24 24

Direct

0.0000000000000000	0.0000000000000000	0.7682361706644423
0.0000000000000000	0.0000000000000000	0.8842248181204013
0.0000000000000000	0.0000000000000000	0.4197004282485300
0.0000000000000000	0.0000000000000000	0.5361785877428379
0.0000000000000000	0.0000000000000000	0.6521937366846079
0.0000000000000000	0.0000000000000000	-0.0007516541425205
0.0000000000000000	0.4999998767678591	0.8262325836857310
0.0000000000000000	0.4999998767678591	0.3631628255710889
0.0000000000000000	0.4999998767678591	0.9427107431800394
0.0000000000000000	0.4999998767678591	0.4781863247367472
0.0000000000000000	0.4999998767678591	0.5941750007641338
0.0000000000000000	0.4999998767678591	0.7102174347439610
0.5000001232321409	-0.0000000000000000	0.8262325836857310
0.5000001232321409	0.0000000000000000	0.3631628255710889
0.5000001232321409	-0.0000000000000000	0.9427107431800394
0.5000001232321409	0.0000000000000000	0.4781863247367472
0.5000001232321409	0.0000000000000000	0.5941750007641338
0.5000001232321409	-0.0000000000000000	0.7102174347439610
0.5000001232321409	0.4999998767678591	0.7682361706644423
0.5000001232321409	0.4999998767678591	0.8842248181204013
0.5000001232321409	0.4999998767678591	0.4197004282485300
0.5000001232321409	0.4999998767678591	0.5361785877428379
0.5000001232321409	0.4999998767678591	0.6521937366846079
0.5000001232321409	0.4999998767678591	-0.0007516541425205
0.0000000000000000	-0.0000000000000000	0.8262465426300881
-0.0000000000000000	-0.0000000000000000	0.3612255449924354
-0.0000000000000000	-0.0000000000000000	0.9423474029623579
-0.0000000000000000	-0.0000000000000000	0.4781431081986664
-0.0000000000000000	0.0000000000000000	0.5941806340689756
-0.0000000000000000	-0.0000000000000000	0.7102352622626177
0.0000000000000000	0.4999998767678591	0.7682305373596005
-0.0000000000000000	0.4999998767678591	0.8842680346584832
0.0000000000000000	0.4999998767678591	0.4200637684662109
-0.0000000000000000	0.4999998767678591	0.5361646287984808
0.0000000000000000	0.4999998767678591	0.6521759091659513
0.0000000000000000	0.4999998767678591	0.0011856264361339
0.5000001232321409	-0.0000000000000000	0.7682305373596005
0.5000001232321409	0.0000000000000000	0.8842680346584832
0.5000001232321409	-0.0000000000000000	0.4200637684662109
0.5000001232321409	0.0000000000000000	0.5361646287984808
0.5000001232321409	-0.0000000000000000	0.6521759091659513
0.5000001232321409	-0.0000000000000000	0.0011856264361339
0.5000001232321409	0.4999998767678591	0.8262465426300881
0.5000001232321409	0.4999998767678591	0.3612255449924354
0.5000001232321409	0.4999998767678591	0.9423474029623579
0.5000001232321409	0.4999998767678591	0.4781431081986664
0.5000001232321409	0.4999998767678591	0.5941806340689756

0.5000001232321409 0.4999998767678591 0.7102352622626177

LiF_110_SURFACE

1.0000000000000000

4.0573829999999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.7380069999999996 0.0000000000000000
0.0000000000000000 0.0000000000000000 35.0000000000000000

Li F
24 24

Direct

-0.0000000000000000 0.0000000000000000 0.7539658695759227
0.0000000000000000 0.0000000000000000 0.8360402494051985
0.0000000000000000 0.0000000000000000 0.9172863988498324
0.0000000000000000 0.0000000000000000 0.5864787195848863
-0.0000000000000000 0.0000000000000000 0.6712984663294859
0.0000000000000000 0.0000000000000000 -0.0043134653517935
-0.0000000000000000 0.5000000871382682 0.7539658695759227
0.0000000000000000 0.5000000871382682 0.8360402494051985
0.0000000000000000 0.5000000871382682 0.9172863988498324
0.0000000000000000 0.5000000871382682 0.5864787195848863
-0.0000000000000000 0.5000000871382682 0.6712984663294859
0.0000000000000000 0.5000000871382682 -0.0043134653517935
0.5000001232321409 0.2500000435691376 0.7951907589955086
0.5000001232321409 0.2500000435691376 0.8778581622419455
0.5000001232321409 0.2500000435691376 0.5534700939232243
0.5000001232321409 0.2500000435691376 0.9626778804151100
0.5000001232321409 0.2500000435691376 0.6318702297215989
0.5000001232321409 0.2500000435691376 0.7131163505947978
0.5000001232321409 0.7499999564308624 0.7951907589955086
0.5000001232321409 0.7499999564308624 0.8778581622419455
0.5000001232321409 0.7499999564308624 0.5534700939232243
0.5000001232321409 0.7499999564308624 0.9626778804151100
0.5000001232321409 0.7499999564308624 0.6318702297215989
0.5000001232321409 0.7499999564308624 0.7131163505947978
0.0000000000000000 0.2500000435691376 0.7951869929756007
0.0000000000000000 0.2500000435691376 0.8774867084576480
-0.0000000000000000 0.2500000435691376 0.5495487381283426
-0.0000000000000000 0.2500000435691376 0.9604877308430558
0.0000000000000000 0.2500000435691376 0.6309728347289643
-0.0000000000000000 0.2500000435691376 0.7129826000781684
0.0000000000000000 0.7499999564308624 0.7951869929756007
0.0000000000000000 0.7499999564308624 0.8774867084576480
-0.0000000000000000 0.7499999564308624 0.5495487381283426
-0.0000000000000000 0.7499999564308624 0.9604877308430558
0.0000000000000000 0.7499999564308624 0.6309728347289643
-0.0000000000000000 0.7499999564308624 0.7129826000781684
0.5000001232321409 0.0000000000000000 0.7539696355958306
0.5000001232321409 0.0000000000000000 0.8361739999218279
0.5000001232321409 0.0000000000000000 0.9181837938424671
0.5000001232321409 0.0000000000000000 0.5886688691569405
0.5000001232321409 0.0000000000000000 0.6716699201137833

0.5000001232321409	0.0000000000000000	-0.0003921095569116
0.5000001232321409	0.5000000871382682	0.7539696355958306
0.5000001232321409	0.5000000871382682	0.8361739999218279
0.5000001232321409	0.5000000871382682	0.9181837938424671
0.5000001232321409	0.5000000871382682	0.5886688691569405
0.5000001232321409	0.5000000871382682	0.6716699201137833
0.5000001232321409	0.5000000871382682	-0.0003921095569116

LiF_111_SURFACE

1.0000000000000000

5.7380069999999996 0.0000000000000000 0.0000000000000000

2.8690030000000002 4.9692590000000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 35.0000000000000000

Li F
28 28

Direct

1.0005263564594800	0.0005265307360168	0.7996672513545068
0.9997649347023175	-0.0002348910211463	0.5972309768782608
0.6623970450876734	0.1623969968637563	0.8662864737583906
0.6683417238618468	0.1683416756379305	0.6652257246808396
0.5005264067687843	0.5005264301173963	0.7996672513545068
0.4997649850116214	0.4997650083602334	0.5972309768782608
0.4983247361927593	-0.0016751766689727	0.7993385610334421
0.5042694149669336	0.0042695021052014	0.5982778119558911
0.3333333423202234	0.3333331991751720	0.7322821428571444
0.3542652686530106	0.3542651255079592	0.9407673896775204
0.3124014159874361	0.3124012728423848	0.5237968960367685
0.1623971690549136	0.6623970974823842	0.8662864737583906
0.1683418478290878	0.6683417762565576	0.6652257246808396
0.1669015253522898	0.1669013899901044	0.8673333088360210
0.1661401035951267	0.1661399682329412	0.6648970343597750
0.9983247865020637	0.4983247227124065	0.7993385610334421
1.0042694652762392	0.5042694014865807	0.5982778119558911
0.8333332920109200	0.8333332997937930	0.7322821428571444
0.8542652183437084	0.8542652261265814	0.9407673896775204
0.8124013656781316	0.8124013734610046	0.5237968960367685
0.8333332551819552	0.3333331991751720	0.7322821428571444
0.8169088302158586	0.3169087742090738	0.9281044478120890
0.8497576801480520	0.3497576241412702	0.5364598379021999
0.6669014750429861	0.6669014906087322	0.8673333088360210
0.6661400532858227	0.6661400688515687	0.6648970343597750
0.3333333791491881	0.8333332997937930	0.7322821428571444
0.3169089541830900	0.8169088748276964	0.9281044478120890
0.3497578041152863	0.8497577247598896	0.5364598379021999
0.9985985529926331	-0.0014012727308310	0.8970695775410269
0.9998394781451055	-0.0001603475783593	0.6989843979439646
0.6660128669169345	0.1660131205488727	0.7662369531445955
0.6776456522333071	0.1776459058652456	0.5603154891152378
0.6836255876362956	0.1836258412682347	0.9616038858265283
0.4985986033019359	0.4985986266505478	0.8970695775410269
0.4998395284544074	0.4998395518030194	0.6989843979439646

0.4890207072026934	-0.0109792056590386	0.9042487965990511
0.4830407717997035	-0.0169591410620279	0.5029603713163326
0.5006534925190658	0.0006535796573341	0.6983273325696934
0.3300044128087543	0.3300042696637033	0.8337533093319419
0.3366622718316921	0.3366621286866407	0.6308109763823398
0.1660130915027810	0.6660130199302521	0.7662369531445955
0.1776458768191539	0.6776458052466247	0.5603154891152378
0.1836258122221429	0.6836257406496131	0.9616038858265283
0.1668268812908960	0.1668270477845664	0.7655798877703243
0.1680678064433679	0.1680679729370383	0.5674947081732620
0.9890207575119966	0.4890206937223406	0.9042487965990511
0.9830408221090079	0.4830407583193506	0.5029603713163326
1.0006535428283680	0.5006534790387129	0.6983273325696934
0.8300043624994503	0.8300043702823233	0.8337533093319419
0.8366622215223897	0.8366622293052627	0.6308109763823398
0.8332876760230321	0.3332876200162483	0.8325138875924367
0.8333788343408783	0.3333787783340957	0.6320503981218450
0.6668269316001981	0.6668269471659442	0.7655798877703243
0.6680678567526716	0.6680678723184176	0.5674947081732620
0.3332877999902644	0.8332877206348699	0.8325138875924367
0.3333789583081119	0.8333788789527161	0.6320503981218450

Li2V02F_100_SURFACE

1.0000000000000000

8.875391999999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.8763810000000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	50.0000000000000000

V	Li	O	F
28	56	56	28

Direct

0.8335014525816370	0.0000000000000000	0.9370991218901933
0.6562678139020874	0.8750016755548345	0.8956215259541541
0.6562678139020874	0.1249984086459012	0.8956215259541541
0.4865525797956154	0.7499902361859868	0.8534714531443476
0.4865525797956154	0.2500098480147480	0.8534714531443476
0.4865470239709472	0.0000000000000000	0.8534681196110919
0.3209130264050933	0.3749841675399717	0.8115016495556433
0.3209130264050933	0.6250158324600282	0.8115016495556433
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32 160 64 128

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