

Vibrational Study of Iodide-Based Room-Temperature Ionic-Liquid Effects on Candidate N719-Chromophore/Titania Interfaces for Dye-Sensitised Solar-Cell Applications from Ab-Initio based Molecular-Dynamics Simulation

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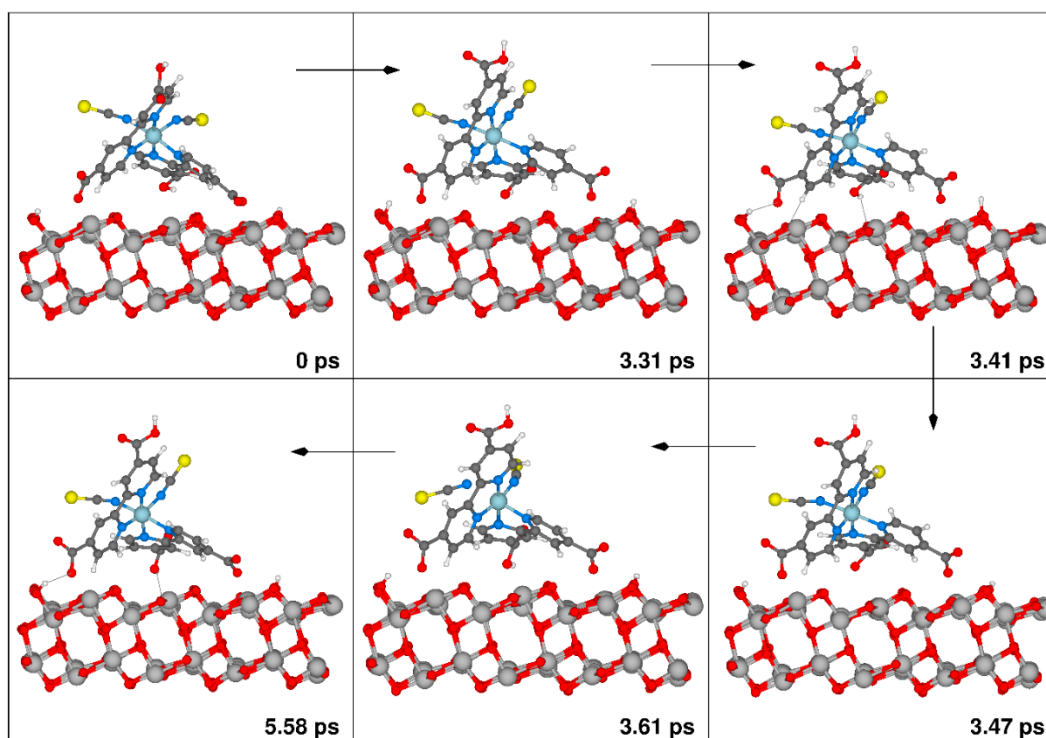


Figure S1. Snapshots of a typical trajectory showing some lowest energy structures of PBE system II. Atom labeling can be seen in Figure 1.

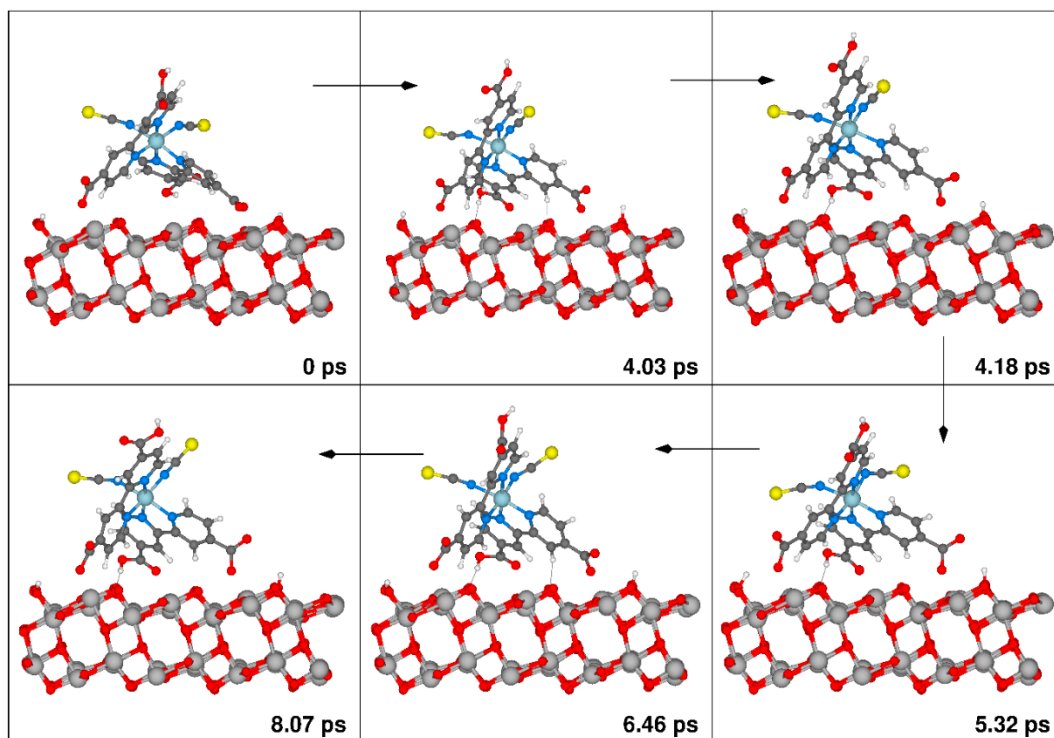


Figure S2. Snapshots of a typical trajectory showing some lowest energy structures of BLYP system II. Atom labeling can be seen in Figure 1.

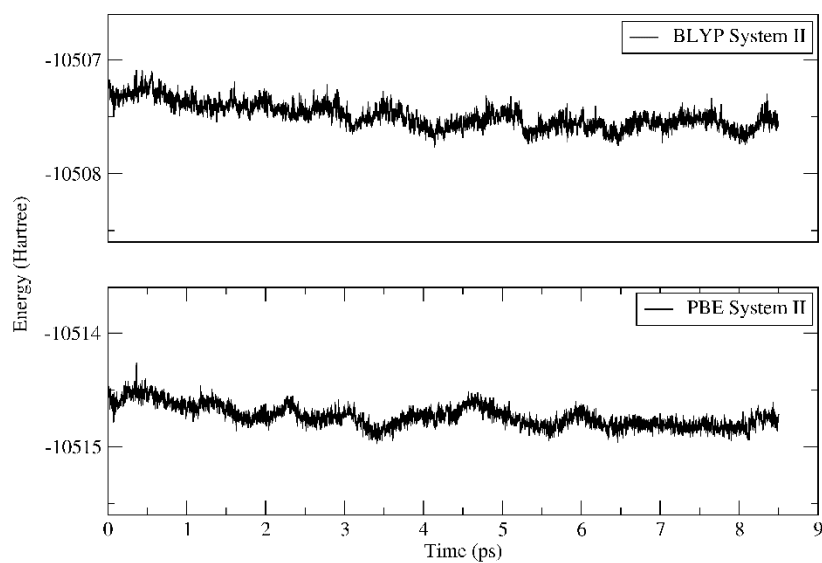


Figure S3. Energy conservation graph of BLYP system II (top) and PBE system II (bottom).

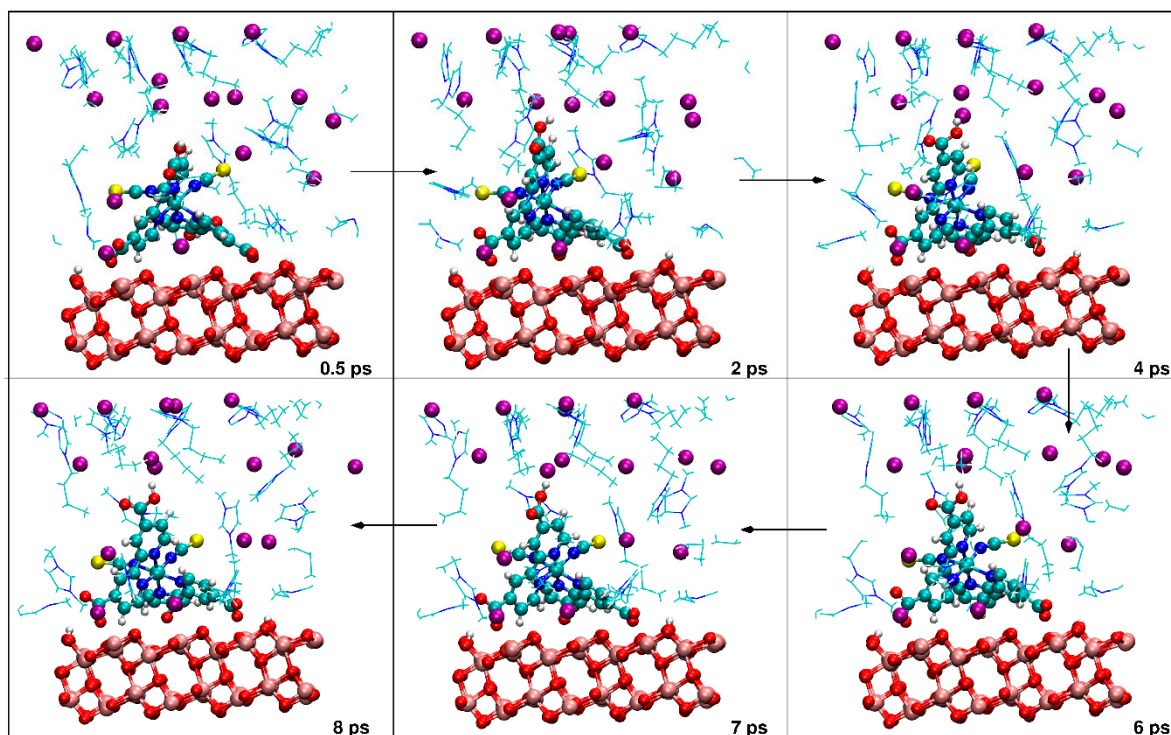


Figure S4. Snapshots of a typical trajectory showing with I[bmim]⁺. Carbon is shown in cyan, nitrogen in blue, oxygen in red, hydrogen in white, titanium in light pink, sulphur in yellow, ruthenium in light cyan, surrounded by nitrogens and iodine in purple. Ionic liquid(bmim) shown in wired form for ease of viewing.

Cp2k Input Sample Script

&GLOBAL

PROJECT Sample_System

RUN_TYPE MD

PRINT_LEVEL Medium

WALLTIME 1100

&END GLOBAL

&MOTION

&CONSTRAINT

&FIXED_ATOMS

LIST 25 31 37 43 49 55 61 67 73 79

LIST 85 91 97 98 99 100 101 102 103

LIST 104 105 106 107 108 109 110 111

LIST 112 113 114 115 116 117 118 119

LIST 120 121 122 123 124 125 126 127

LIST 128 129 130 131 132 133 134 135

LIST 136 137 138 139 140 141 142 143

LIST 144 169 175 181 187 193 199 205

LIST 211 217 223 229 235 241 242 243

LIST 244 245 246 247 248 249 250 251

LIST 252 253 254 255 256 257 258 259

LIST 260 261 262 263 264 265 266 267

LIST 268 269 270 271 272 273 274 275

LIST 276 277 278 279 280 281 282 283

LIST 284 285 286 287 288

&END FIXED_ATOMS

&END CONSTRAINT

&MD

ENSEMBLE NVT

STEPS 2

TIMESTEP 1

TEMPERATURE 300.0

&THERMOSTAT

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    TIMECON 150.0
      LENGTH 3
      YOSHIDA 3
      MTS 2
    &END NOSE
  &END THERMOSTAT
&END MD

&END MOTION

&FORCE_EVAL
  METHOD Quickstep
  &DFT

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    POTENTIAL_FILE_NAME NEWPOT
    &MGRID
      CUTOFF 400
    &END MGRID
    &QS
      EPS_DEFAULT 1.0E-14
      EXTRAPOLATION ASPC
      EXTRAPOLATION_ORDER 3
    &END QS
```

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  MAX_SCF 4
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  MINIMIZER CG
  LINESEARCH 3PNT
PRECONDITIONER FULL_SINGLE
  &END OT
  &OUTER_SCF ON
  EPS_SCF 1.0E-5
MAX_SCF 4
  &END OUTER_SCF
  SCF_GUESS RESTART

  &END SCF

&PRINT
&END
&XC
  &XC_FUNCTIONAL PBE
  &END XC_FUNCTIONAL
&END XC
&END DFT
&SUBSYS
&CELL
  ABC 22.69 20.45 25.927
&END CELL
&COORD
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Ti	18.8574152544	15.4482197275	-0.3727509286
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Ti	1.8537971514	2.8931184270	-0.9382277155
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Ti	7.5236153776	18.2561226021	-0.8718755670
O	7.6215962507	18.7514117831	-2.7814109486
O	7.5328373403	20.1578576587	-0.1675867966
O	5.6671836321	18.5564421525	-0.8500725163
Ti	5.6169549445	1.6773090099	-3.9985636832
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Ti	13.1124969439	4.3851787763	-4.5199802408
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Ti	16.9147927707	4.4159559067	-4.4649384804
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Ti	0.0390508159	19.5813592385	-4.4623676922
O	-0.0075015484	1.2186056215	-3.8665132980
O	-1.8908083637	20.1356723583	-4.6785322675
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O	3.7325109843	18.1457057086	-5.3417236308
Ti	3.8613942864	19.6994072989	-4.3667397079
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O	1.7654553093	6.3404773357	-4.0253616092
Ti	1.7237927197	4.3515552032	-4.4109580068
O	3.6343814433	4.8027083282	-4.5813495404
O	1.7221686055	2.7712312696	-5.4071269109
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O	5.6912386092	20.2227168458	-4.5713546350
O	5.5732396332	6.3921582062	-4.1051736891
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O	5.5944355156	2.8494353937	-5.3795779632
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H	14.3615992547	10.4189958967	9.1514237327
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C	14.6136317574	16.0299916222	14.6758069484
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C	15.7367785479	15.3034209766	15.6071411300
H	14.2195540368	16.8742163420	15.1939312703
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N	3.4888558088	14.4961440360	5.8633871620
C	3.3403362328	14.9241204870	7.1641294123
N	4.4871851653	14.7550737356	7.7791451077
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H	2.3884969281	15.3644674432	7.5748086006
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C	4.8578582809	13.5135722708	11.2804231801
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C	10.1801773962	21.2999673875	10.3927473927
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H	11.8755138266	18.3383794053	15.2213813608
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N	2.3249443399	9.5747604505	8.4316551289

S	2.6123683911	8.1693522904	9.0868200473
O	3.8174892766	8.1323572966	9.9090832581
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F	0.8647002093	6.7100293174	10.2084580526
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S	2.5746834015	11.0350540858	8.8701684882
O	3.6182520613	11.7244445776	8.0644185429
O	2.5108672591	11.3190015373	10.3085176382
C	1.0133610853	11.8758387344	8.1352008832
F	1.1293014049	13.2354143795	8.2247826655
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F	0.9000815053	11.5401577639	6.7812569393
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S	0.4207450129	16.2288669088	16.0878303389
O	0.8069344244	15.2080227076	15.1699264241
O	1.3158476332	17.1167957004	16.7634165487
C	-0.8392360013	17.2562128067	15.1525669118
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F	-1.8186374331	17.7880819218	15.8955415091
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S	-0.4168143882	14.9402480175	18.4765678423
O	-1.5368114247	15.2848036405	19.4027805606
O	0.9526733963	15.0705979780	19.0959628014
C	-0.5487520594	13.0599275076	17.9470721598
F	-1.8552313981	12.7985887450	17.8052679773

F	-0.0414983384	12.1802614867	18.8030821194
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N	3.8048456912	6.3639599349	2.9572666381
S	3.4899193222	7.6723435370	3.8481066238
O	3.7026545620	8.8604452729	2.9926229988
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C	1.6323278778	7.6070958767	3.7818305300
F	0.9955895411	8.1853450394	4.8498233111
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S	4.4245022809	5.0847417398	3.5915851563
O	4.4620417668	4.0944867689	2.5459216212
O	3.9922063550	4.6385863048	4.8788936558
C	6.2480409508	5.5088489305	3.8849068403
F	6.6598395503	5.3456918501	5.1780002263
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F	7.0536340443	4.6907123182	3.1612362228
N	10.6999957565	8.3034810237	14.9612079143
S	12.0998026284	7.8610583708	15.4046462576
O	13.2334144546	8.2390485421	14.6499940863
O	12.0128019554	6.4566403946	15.8281128213
C	12.2326700547	8.6478212177	17.0938712689
F	13.3614659491	8.2666507336	17.7547951513
F	12.3568109814	10.0105127858	16.9865541037
F	11.2000881870	8.4432782342	17.9360377951
S	10.2552003843	9.6546448803	14.2011759146
O	11.3148493190	10.6466749280	14.1727092989

O	8.9169648274	9.9138025177	14.6322861668
C	10.0050542898	9.0857123039	12.4766202529
F	9.2823591969	9.9933419411	11.8043539408
F	9.3777590599	7.9164411876	12.4668441890
F	11.1637204334	8.9466983631	11.8575966986
N	24.5406802590	25.8602363691	14.5165846804
S	23.8326611105	24.4081479283	14.5646830045
O	22.3822197983	24.2928810499	14.5679841360
O	24.6009408042	23.4987522098	15.3627483690
C	24.3156211123	23.8724414774	12.7780428583
F	25.6775042297	23.7548986629	12.7532882642
F	23.8923353114	22.5947534566	12.4587355145
F	23.9680983531	24.7029311934	11.7944113012
S	24.7104448688	26.6266185609	15.9348125354
O	26.0872203915	26.7600343509	16.4061619976
O	23.7163687893	26.3915725105	17.0122369891
C	24.3334140951	28.4141145307	15.3887133566
F	23.3411315846	28.5340595737	14.4929245870
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F	23.9630904940	29.0819556005	16.5105430737
N	12.3986850210	1.6945152287	6.4313126599
S	11.9607792479	0.2999336029	7.0318636620
O	10.4781393678	0.2304423439	7.1525285245
O	12.7353290584	-0.3451818860	8.1031696501
C	12.3867262295	-0.7737930294	5.5313312611
F	13.6910072917	-0.6960784369	5.2129426901
F	12.1297481014	-2.0217774181	5.8526475953

F	11.7172647309	-0.3801410660	4.4097559402
S	12.3157748250	3.0713355058	7.2336438765
O	13.2255968625	4.0493666640	6.6301183246
O	12.2849405916	2.9158688811	8.6642973511
C	10.5832820793	3.7069281405	6.7866897633
F	10.5404153911	5.0323388359	6.7766779145
F	9.7115509436	3.2736092049	7.7416975073
F	10.2267691311	3.2392828845	5.5626275956
N	19.5544346985	11.2427736785	12.9357219354
S	19.7319756944	11.9411959702	11.5067527400
O	20.0413462084	10.9239885252	10.4978775083
O	20.4105010714	13.2415498584	11.3636750838
C	18.0251026508	12.5279043516	11.0428770707
F	17.7163061681	13.6310988302	11.7431284460
F	18.1271063714	12.9651950565	9.7296381180
F	17.0343957930	11.6168557323	11.0670687646
S	20.0727932430	11.8016180497	14.3400598920
O	21.1486156622	12.7777270547	14.2408902558
O	20.1824724904	10.6763166675	15.2554912523
C	18.5993745688	12.8794571592	14.8891685089
F	18.6831407598	14.1512973431	14.4147704434
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S	7.5590081490	16.6402315531	5.1605858659
O	7.4922469075	15.2000269434	5.1743294843
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C	9.3370496430	17.1407668218	4.6789668560
F	9.3588288514	18.0937507834	3.6780521366
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S	6.0733169152	18.6238729086	3.9924558644
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O	6.6986101806	19.5384946282	4.9647629540
C	4.2814584290	18.6033919098	4.5220992514
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S	19.3161616290	12.1099199780	3.8444153293
O	19.3509683438	12.5781662460	5.2412467492
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C	20.9915830296	11.1393584738	3.7366747757
F	20.8955384759	10.0008831848	3.0162015921
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F	21.2297988044	10.7198994185	5.0274472673
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O	17.0110246747	11.2336571609	5.6406556657
O	16.8854802556	9.0079382360	4.3702802270
C	15.6077665433	10.9592813518	3.4160938499
F	15.5432432168	12.3274298193	3.1460949376
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C	19.1013276469	17.7931877394	8.2112737197
F	18.4262115278	17.3849819028	7.0796194659
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O	19.6989480127	22.2211214346	9.8399603092
O	20.1723282913	22.7221090127	7.4603881799
C	21.9017930493	21.2714164042	8.5917645904
F	22.1935472523	20.6845343606	7.3838232960
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S	5.0465754719	17.1612217140	13.7252555300
O	6.5109998652	17.3323700439	13.7619640344
O	4.5806963793	16.5457334246	12.4631068687
C	4.7081159093	15.9928501992	15.1229796694
F	5.5813461840	16.1981838652	16.1090996815
F	3.4783519005	16.0827222984	15.5740644952
F	4.8999089415	14.7286577334	14.5899789505
S	4.6200679046	19.3932623843	15.2221147785
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O	4.1301361393	19.0495908458	16.5222105673
C	3.4226228202	20.7644186207	14.8274915014
F	2.1487155014	20.3459415227	14.8081111954

F	3.7052115244	21.2267766363	13.6018594981
F	3.5601876517	21.7029372969	15.8050720189
N	16.3447603734	3.9324142932	11.3390954186
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O	15.9127369123	3.1941739848	13.6922735284
C	15.7103175039	1.4457217516	11.7672840050
F	16.9859726273	1.1322356208	11.8642565862
F	14.9476997504	0.5377715363	12.5785147932
F	15.3169932151	1.2852069287	10.4886718986
S	15.8455996991	5.1357956020	10.3670205647
O	14.4377009029	5.1097102266	10.0294990016
O	16.8546993384	5.3851533968	9.3982186289
C	16.1063708235	6.5113494281	11.6561737430
F	17.3512967379	6.4260996141	12.1194734434
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Sample input file for CP2K:

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&KIND H
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  POTENTIAL GTH-PBE-q1
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&END KIND
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&KIND C
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POTENTIAL GTH-PBE-q4
&END KIND
&KIND N
BASIS_SET TZVP-MOLOPT-GTH
POTENTIAL GTH-PBE-q5
&END KIND
&KIND CI
    BASIS_SET TZV2P-MOLOPT-GTH
    POTENTIAL GTH-PBE-q7
&END KIND
&KIND Ti
    BASIS_SET TZVP-GTH-PBE-q12-g7-confined
    POTENTIAL GTH-PBE-q12
&END KIND
&KIND S
    BASIS_SET TZVP-MOLOPT-GTH
    POTENTIAL GTH-PBE-q6
&END KIND
&KIND O
    BASIS_SET TZVP-GTH
    POTENTIAL GTH-PBE-q6
&END KIND
&KIND Ru
    BASIS_SET TZVP-GTH-PBE-q16-g6-confined
    POTENTIAL GTH-PBE-q16
&END KIND
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  BASIS_SET TZV2P-MOLOPT-GTH
  POTENTIAL GTH-PBE-q7
&END KIND

&KIND S
  BASIS_SET TZVP-GTH
  POTENTIAL GTH-PBE-q6
&END KIND

&END SUBSYS

&END FORCE_EVAL
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