

Supporting Information for:
Modelling Molecular Crystals by QM/MM: Self-Consistent Electrostatic Embedding
for Geometry Optimizations and Molecular Property Calculations in the Solid

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Periodic BP86-D optimized geometries of the cell of **3** and **4** in Cartesian coordinates
(Å):

Molecule **3**:

O	-0.852611061294	6.821219190032	10.758448668658
O	1.650815116599	6.953800691535	6.246473370184
O	5.940958374315	2.279021771562	0.526034949617
O	3.374659925513	2.278419944483	5.112968550640
O	4.121265483665	6.972264577133	10.681219963997
O	6.611598442004	6.868207831148	6.161881807057
O	10.907384725902	2.345308597375	0.574043347234
O	8.428533020827	2.366886842506	5.032452162049
Cl	1.436102349517	5.120053843795	9.760053013019
Cl	1.349875291417	6.833689869402	12.838859099446
Cl	1.345856749138	8.673219241127	9.823984286721
Cl	3.927609094029	8.713259253358	7.174920637727
Cl	3.811440214553	6.954024702107	4.122664321008
Cl	3.907713014959	5.158507794616	7.155778278226
Cl	3.676001333459	4.068505622593	1.440193253412
Cl	3.756326479278	2.258835053259	-1.580333858478
Cl	3.666299719796	0.523156644831	1.480595341400
Cl	1.113416077203	0.530599668106	4.126946860485
Cl	1.172679985968	2.273387395620	7.194514864752
Cl	1.145298664986	4.084720824235	4.166780655809
Cl	6.365655706914	5.139724849843	9.805585698738
Cl	6.257103318881	6.913817406817	12.841998036456
Cl	6.464421719275	8.684282126691	9.809422522760
Cl	8.861598622737	8.668781062992	7.084728931590
Cl	8.810512845978	6.846702145808	4.069850115519
Cl	8.884763877143	5.124411180594	7.140918414632
Cl	8.644488619212	4.101735198899	1.538593973739
Cl	8.732962547824	2.386234848677	-1.535567984044
Cl	8.651196381180	0.548125046068	1.479410338968
Cl	6.178286682630	0.543496801598	4.149453425251
Cl	6.287985437891	2.328870927236	7.183812453596
Cl	6.098870208951	4.087981479486	4.143668233233
V	0.723431365388	6.860766364675	10.787072937366
V	3.226479666484	6.945226658809	6.185776997842
V	4.364442289412	2.282503237941	0.475866482572
V	1.798167719432	2.290757526563	5.142318092706
V	5.695738924740	6.930900816112	10.772622927953
V	8.188276531789	6.875962702160	6.121766210954
V	9.331414752867	2.343513787121	0.523740820460
V	6.853510222966	2.333837517349	5.115839900126

Molecule 4:

O	1.064820714163	5.187187344484	4.999914785424
O	4.496918253188	3.679743451242	6.985827267877
O	1.969771519515	5.677995777679	2.449728099633
O	3.590006077988	3.200053987523	9.538500442700
O	2.524781411053	8.354897721611	3.390778464886
O	3.020065780605	0.523507939984	8.599537532938
O	0.174982881916	7.340828748935	3.746991621969
O	5.376330035313	1.524943086376	8.247331617931
O	1.611611254948	-0.771321333887	6.698738754828
O	3.944758513284	9.640957683931	5.292070431649
C	2.717938164867	4.702127247339	1.956046223967
C	2.839258806776	4.172662601313	10.034330913774
C	2.350519661481	4.098138764810	0.732435832395
C	3.203798120672	4.773776621217	11.260297429682
C	3.141746600590	3.097106344689	0.178046226750
C	2.409594991398	5.771284129895	11.816856803351
C	4.326773802568	2.674785120188	0.811754554356
C	1.224910573797	6.193565563552	11.182450980497
C	4.714502975611	3.280390314123	1.999557936245
C	0.840212021569	5.591036239694	9.992160483442
C	3.926943335003	4.296717457007	2.594319789317
C	1.630157122855	4.577520949316	9.395764779164
C	4.408951213333	4.967896453056	3.770938733317
C	1.149026982256	3.906297516422	8.218930711735
C	4.403170507067	6.506373886236	5.590764096653
C	1.153855363499	2.365266818311	6.401255614216
C	3.357586506495	6.691701493544	6.674147625544
C	2.197923156963	2.177178644415	5.317008353557
C	1.521889309849	9.061080609066	2.900294671854
C	4.018265333488	-0.186602578080	9.093947059729
C	1.630003973344	10.307007615692	2.252288429609
C	3.901359932948	-1.430818644272	9.743367468610
C	1.246561012725	0.206816315268	1.701203097668
C	4.280211151145	8.663288524433	10.297295284094
C	5.994865668627	10.300177045864	1.818583310492
C	-0.464488033895	-1.437443342927	10.181686565920
C	5.841121437775	9.107545543489	2.534529981369
C	-0.302166594556	-0.246330569974	9.464919655295
C	0.211842470331	8.497412205572	3.063478317836
C	5.331704771053	0.369804184242	8.933044482564
C	1.070799750675	7.503832990017	7.028372966294
C	4.484465653253	1.365181583779	4.961439938463
C	0.149104673606	8.673819333237	6.705665724038
C	5.406828296229	0.196122835249	5.284852599911
H	1.456456791327	4.460583454737	0.228999814110
H	4.097701986367	4.411335836215	11.764005393766
H	2.411054706078	0.848796935637	11.223966910378

H	3.137598757841	8.016759747737	0.773015934236
H	4.944495040652	1.907207517667	0.345088588995
H	0.605045719936	6.958625481584	11.650353363359
H	5.641588600949	2.985376423987	2.494937998651
H	-0.086939647003	5.885571555246	9.496618691350
H	5.435188805655	4.735898281381	4.086053223345
H	0.122274779938	4.136469719896	7.904271596614
H	4.751006079506	7.490621739622	5.249328875399
H	0.805967286427	1.382028033767	6.745730952505
H	5.262048196315	5.921308170329	5.948015321732
H	0.294978768795	2.950167363293	6.043936683453
H	3.008962318458	5.717631045974	7.040643187723
H	2.546291671432	3.150389992874	4.947994493642
H	3.746416885025	7.282618570981	7.518473994940
H	1.807813811151	1.584608409915	4.474431772324
H	3.361319108674	0.090068749663	2.153129770999
H	2.166966923233	8.792036338132	9.840247444044
H	1.350990754057	1.150783905446	1.163440801078
H	4.169669552855	7.720192788739	10.835343779517
H	5.893943244442	0.077938389964	1.342699404137
H	-0.367243277207	8.779989061444	10.659573501267
H	4.855740700723	8.641394556601	2.680138723636
H	0.685983143640	0.214492329770	9.320408725295
H	0.523231615790	6.551747628308	7.011660023820
H	5.031610936500	2.317526280285	4.976826113581
H	1.488109426080	7.641999645329	8.041699420248
H	4.066094699753	1.226579530640	3.948623210739
H	-0.283683701765	8.568285872426	5.706200758018
H	5.839169186065	0.301825999275	6.284595464564
H	-0.672513047948	8.690903863702	7.443078835887
H	6.228611541315	0.178713938570	4.547654709620
H	2.518458347276	8.362646904020	5.853534793424
H	3.038841747124	0.507805112241	6.139795260653
H	1.933076979991	-0.513978410087	7.603019829553
H	3.618801301745	9.386593742045	4.388521251556
N	3.744268343347	5.845277272502	4.458465932096
N	1.814145533122	3.029218923558	7.531328382051
N	2.201580094003	7.402627903461	6.063450492615
N	3.354725807548	1.467550837867	5.927486233788
V	1.716584539436	6.404147172727	4.169276311291
V	3.840023742979	2.468223618465	7.820675850025

QM/MM-NPA optimized geometries of the larger QM regions of molecules **1-4** in Cartesian coordinates (Å):

1 (B3PW91/aug-cc-pVTZ):

B	1.82077898	2.54672275	-4.00274589
C	0.36998120	4.09500936	-2.25580140

F	1.66578313	3.08307214	-5.25445929
F	3.11505902	2.59346244	-3.55461665
F	1.28489799	1.27408893	-3.89605857
H	-0.19579247	4.67542866	-1.54562600
N	0.95311866	3.46757231	-3.00007075
B	1.92720239	1.97452481	-8.45972322
C	0.80462268	0.16832608	-6.72870596
F	1.85112358	1.43686410	-9.72238938
F	3.21653662	2.08448332	-7.99660114
F	1.19981677	3.14856191	-8.32653836
H	0.46433641	-0.55436895	-6.01644621
N	1.20903775	0.91793855	-7.49045313
B	2.64862219	-1.72952545	-4.19209230
C	4.08840812	-0.25869742	-2.35931583
F	2.89391371	-1.08010087	-5.38587836
F	1.33327361	-1.64350813	-3.79087542
F	3.10146617	-3.02531169	-4.18744849
H	4.65287976	0.34742154	-1.65849973
N	3.51525848	-0.92189846	-3.09661859
B	6.52592117	1.98962596	-4.61319571
C	5.32884046	0.24130757	-6.36745263
F	6.38451517	1.40547264	-3.37697638
F	7.83129087	2.07215345	-5.02659959
F	5.83745795	3.18392359	-4.74026305
H	4.92236875	-0.46655117	-7.05807516
N	5.81094670	0.97934549	-5.64097666
B	-2.04865776	6.16018699	-4.57918191
C	-0.57628219	4.63687966	-6.35664457
F	-1.98341743	5.48013068	-3.37960822
F	-3.31235348	6.20660068	-5.11234817
F	-1.46230132	7.40335887	-4.50137494
H	-0.00808555	4.03714893	-7.05842155
N	-1.17021257	5.29241187	-5.62855455
B	2.53528046	6.12153887	-8.52188858
C	4.07474088	4.62228869	-6.78859752
F	2.63189584	5.48341274	-9.73704977
F	1.27615401	6.07504470	-7.97307580
F	3.04691954	7.39690005	-8.55499844
H	4.66148823	4.02797451	-6.09936069
N	3.48721009	5.27398137	-7.52401931
B	6.41817997	2.51402863	-0.35118596
C	5.02545367	4.15208665	-2.08002116
F	6.29921377	3.06234486	0.90020547
F	7.71297977	2.46542242	-0.80546366
F	5.78156988	1.28133460	-0.46321221
H	4.45392369	4.75907711	-2.77168420
N	5.61678360	3.50116103	-1.34678925
B	2.59033150	6.72653444	-4.25444051
C	3.80890962	8.44800797	-2.49501771
F	2.70839088	7.29774936	-5.50380471

F	1.28959076	6.65429381	-3.82596020
F	3.27565613	5.52635110	-4.14410124
H	4.23246710	9.14636153	-1.80446679
N	3.33856036	7.73020261	-3.24925118
B	2.19587958	1.96890502	0.23300520
C	0.75700665	0.34088469	1.93755014
F	2.23627309	1.28696496	-0.96014302
F	3.41776639	2.09853095	0.84543647
F	1.52103448	3.16718614	0.15000172
H	0.24382465	-0.30870937	2.61599078
N	1.32163059	1.03157572	1.22256229
B	-2.48521001	1.86696752	-4.44222298
C	-3.78093550	0.30290158	-6.30910954
F	-2.50398213	1.16527606	-3.25548483
F	-1.23288943	2.00426519	-4.98526703
F	-3.17461943	3.05655306	-4.36341532
H	-4.20961437	-0.30679948	-7.07863672
N	-3.29988794	0.95656115	-5.50391884
B	-1.91497210	-1.76797252	-0.15924238
C	-0.43703925	-0.31863081	-2.00942776
F	-1.66755765	-1.13367676	1.03178305
F	-3.21446094	-1.66064837	-0.59009012
F	-1.46675698	-3.06641524	-0.18507430
H	0.13023599	0.27445737	-2.71978638
N	-1.01890973	-0.95993378	-1.25872256
B	-2.46413232	2.43194954	-0.07321608
C	-3.90943304	3.93463490	-1.85945819
F	-2.63884907	3.05037569	1.14323331
F	-1.16284538	2.50061184	-0.52148714
F	-2.98188951	1.16353366	-0.12576545
H	-4.45130113	4.52889827	-2.56125156
N	-3.34020874	3.29431280	-1.10384269
B	2.46861900	6.30514026	0.08375040
C	3.87478101	4.75786963	1.88732253
F	2.54082753	5.63426628	-1.11213746
F	1.20232166	6.32321291	0.63210985
F	3.05014268	7.54643496	0.04084451
H	4.35769226	4.14383216	2.61955588
N	3.34372479	5.43049214	1.13047874
B	-2.02595039	6.71325344	-0.20395992
C	-0.76581037	8.44725593	-1.91737576
F	-1.90930950	7.27976271	1.04191036
F	-3.31539334	6.64025351	-0.65651733
F	-1.35835127	5.49759586	-0.30112525
H	-0.32435432	9.17189395	-2.56915114
N	-1.25874322	7.71064757	-1.19653849

2b (PBE0-D/def2-TZVPP/def2-SVP):

Ru	-2.9253435	-5.0949799	4.3805001
C	-3.4093480	-4.9971832	6.4834474

C	-2.2335898	-4.2451978	6.2513451
C	-2.3136300	-3.0933416	5.4509699
C	-1.1283269	-2.3262320	5.0542040
C	-1.2776647	-1.1540238	4.2980817
C	-0.1701030	-0.3807427	3.9552794
C	1.1069652	-0.7637145	4.3658841
C	1.2723669	-1.9442123	5.0972198
C	0.1694598	-2.7186560	5.4346469
C	-4.1435237	-4.1050255	2.8688397
C	-3.8564186	-2.7877896	2.2382683
C	-4.9602523	-4.3521812	4.0202261
C	-5.7719772	-3.3409771	4.7498009
C	-5.0011350	-5.7838138	4.2345561
C	-5.7984070	-6.5187709	5.2500327
C	-4.2720530	-6.4068874	3.1694857
C	-4.1120073	-7.8665292	2.9601275
C	-3.7503356	-5.3886149	2.3289138
C	-2.9831283	-5.6048687	1.0795669
C	-1.3214146	-7.7087810	5.2039339
C	-0.5646772	-8.8937795	5.5172797
C	-0.2183107	-4.4954614	2.8038509
C	0.9974552	-4.1439767	2.1110518
H	-4.3589990	-4.4804173	6.6162246
H	-3.3244085	-5.9479613	7.0115936
H	-1.2645539	-4.6473744	6.5384965
H	-3.2726541	-2.5729282	5.3814269
H	-2.2769615	-0.8329392	3.9962569
H	-0.2971426	0.5321666	3.3708547
H	1.9699954	-0.1415366	4.1179245
H	2.2658698	-2.2599983	5.4196484
H	0.3328659	-3.6283494	6.0144276
H	-4.5403332	-2.6061765	1.3945354
H	-2.8323832	-2.7510035	1.8387700
H	-3.9837194	-1.9654307	2.9548384
H	-5.4726257	-2.3160368	4.4920460
H	-5.7288616	-3.4444215	5.8426730
H	-6.8305125	-3.4905958	4.4786737
H	-6.7062126	-6.9086517	4.7706197
H	-6.1031194	-5.8646456	6.0702502
H	-5.2364778	-7.3716888	5.6533654
H	-4.2522669	-8.4263163	3.8928347
H	-3.1247938	-8.1030270	2.5392758
H	-4.8825541	-8.1951960	2.2449602
H	-2.4441087	-6.5616948	1.0918835
H	-2.2661253	-4.7960092	0.9094382
H	-3.6848432	-5.5981860	0.2293543
H	0.3476745	-8.8976043	4.9104190
H	-1.1583044	-9.7861587	5.2840834
H	-0.2980426	-8.8838617	6.5825356
H	0.7532448	-3.7922199	1.0982632

H	1.6534749	-5.0233427	2.0401777
H	1.4890769	-3.3355754	2.6745409
N	-1.9260831	-6.7617565	4.9538959
N	-1.1883556	-4.7270645	3.3816251
Ru	0.0107703	-0.1793522	10.3116712
C	0.4948579	-0.2758886	8.2086238
C	-0.6807397	-1.0282882	8.4404158
C	-0.6005272	-2.1803237	9.2405500
C	-1.7857707	-2.9475532	9.6374371
C	-1.6361801	-4.1194760	10.3939434
C	-2.7435516	-4.8929083	10.7370030
C	-4.0207005	-4.5102316	10.3264493
C	-4.1863641	-3.3299353	9.5948954
C	-3.0836438	-2.5554126	9.2570238
C	1.2287425	-1.1694863	11.8234540
C	0.9413414	-2.4864193	12.4545028
C	2.0454608	-0.9229130	10.6718959
C	2.8563588	-1.9347713	9.9422255
C	2.0869868	0.5086952	10.4573145
C	2.8846727	1.2433574	9.4418680
C	1.3579796	1.1322456	11.5221186
C	1.1981275	2.5920516	11.7308373
C	0.8360536	0.1144037	12.3630746
C	0.0692781	0.3312800	13.6125775
C	-1.5930057	2.4350194	9.4893069
C	-2.3488616	3.6205718	9.1758273
C	-2.6962116	-0.7788947	11.8882439
C	-3.9124269	-1.1293898	12.5807478
H	1.4447599	-0.7921032	8.0754041
H	0.4095271	0.6752261	7.6811435
H	-1.6498339	-0.6261263	8.1534146
H	0.3584138	-2.7009135	9.3097542
H	-0.6368736	-4.4402333	10.6960168
H	-2.6162269	-5.8056978	11.3215555
H	-4.8835601	-5.1325444	10.5746948
H	-5.1799632	-3.0143042	9.2725779
H	-3.2472360	-1.6459098	8.6770047
H	1.6256763	-2.6681815	13.2978600
H	-0.0824342	-2.5227761	12.8547153
H	1.0680093	-3.3090055	11.7381025
H	2.5572922	-2.9594546	10.2013208
H	2.8118247	-1.8324696	8.8492747
H	3.9152597	-1.7850818	10.2118674
H	3.7889079	1.6393166	9.9230515
H	3.1955452	0.5872631	8.6255654
H	2.3205804	2.0922308	9.0329771
H	1.3381323	3.1514397	10.7978273
H	0.2110522	2.8287864	12.1518792
H	1.9688473	2.9210476	12.4456504
H	-0.4674519	1.2893887	13.6012082

H	-0.6496142	-0.4760435	13.7819407
H	0.7708813	0.3219560	14.4628673
H	-3.2603061	3.6264678	9.7840293
H	-1.7537518	4.5124690	9.4070671
H	-2.6171324	3.6098209	8.1109882
H	-3.6688300	-1.4809385	13.5937674
H	-4.5676863	-0.2494080	12.6509987
H	-4.4043840	-1.9376060	12.0172820
N	-0.9887146	1.4877053	9.7391815
N	-1.7260608	-0.5476440	11.3105481

3 (BP86-D/def2-QZVPP):

V	0.69269834	-2.30400176	-0.53179298
O	-0.88507825	-2.30400077	-0.59550122
Cl	1.26371896	-2.30400082	1.54298286
Cl	1.38473566	-4.08349318	-1.50587647
Cl	1.38473602	-0.52450738	-1.50587705

4 (BP86/(def2-TZVPP on V,O,N; def2-SVP on C,H)) :

V	2.0777781	-4.4764522	4.1317661
N	4.0807450	-5.1244506	4.3626043
N	2.6522707	-3.5544532	6.0766179
O	1.2779611	-5.5968738	4.9767101
O	2.2230334	-5.2970675	2.4477637
O	2.9593842	-2.5744983	3.3588683
O	0.5817078	-3.4680732	3.6822096
O	1.6265499	-0.9021083	6.7588526
C	2.9701100	-6.2373495	1.8799313
C	2.5374659	-6.8601511	0.6821213
C	3.3659796	-7.7843098	0.0380630
C	4.6289628	-8.1388206	0.5689075
C	5.0625776	-7.5402111	1.7487885
C	4.2469698	-6.5907770	2.4239164
C	4.7452214	-5.9544866	3.6128952
C	4.7663294	-4.5595044	5.5287721
C	3.7437444	-4.3930073	6.6334933
C	2.0042819	-1.8320166	2.8150798
C	2.1750761	-0.6056449	2.1205605
C	1.0501031	0.0660550	1.6061394
C	-0.2546409	-0.4580065	1.7616291
C	-0.4573056	-1.6665089	2.4505321
C	0.6675509	-2.3342065	2.9713309
C	1.5527909	-3.3419699	7.0533790
C	0.7848337	-2.0604557	6.7570422
H	1.5798031	-6.5482985	0.2395175
H	3.0602418	-8.1976167	-0.9315015
H	5.2740130	-8.8414254	0.0240833
H	6.0587046	-7.7633155	2.1658075
H	5.7849926	-6.1924810	3.9039777
H	5.1425169	-3.5609066	5.2336125

H	5.6233875	-5.1903488	5.8259163
H	3.3220931	-5.3661982	6.9461878
H	4.1904407	-3.9030627	7.5253185
H	3.1850805	-0.1899058	1.9771016
H	1.1938680	1.0185114	1.0723022
H	-1.1141689	0.0857656	1.3403932
H	-1.4545592	-2.1040049	2.6120460
H	0.8796686	-4.2228648	7.0299171
H	1.9887829	-3.2907846	8.0765070
H	0.3605296	-2.1008937	5.7370760
H	-0.0635301	-1.9569403	7.4670108
H	3.0542845	-2.6238649	5.8663408
H	2.0238051	-0.7060574	7.6496750
V	4.0998582	2.2232418	7.8737222
N	2.0971094	2.8713936	7.6428072
N	3.5254259	1.3016218	5.9282901
O	4.8996655	3.3432896	7.0284697
O	3.9546549	3.0433775	9.5572874
O	3.2166629	0.3203229	8.6454248
O	5.5950771	1.2136398	8.3227656
O	4.5518144	-1.3508711	5.2452464
C	3.2075359	3.9832879	10.1260241
C	3.6403170	4.6054466	11.3240095
C	2.8114191	5.5287326	11.9689110
C	1.5481116	5.8829698	11.4386207
C	1.1145245	5.2851218	10.2583728
C	1.9304711	4.3364970	9.5824345
C	1.4324790	3.7009153	8.3930876
C	1.4115545	2.3069664	6.4764038
C	2.4341697	2.1405702	5.3716572
C	4.1717089	-0.4222279	9.1894353
C	4.0005358	-1.6485051	9.8839983
C	5.1252419	-2.3204896	10.3987384
C	6.4301100	-1.7967929	10.2434252
C	6.6331838	-0.5883206	9.5545202
C	5.5085968	0.0796605	9.0334967
C	4.6250536	1.0893002	4.9517719
C	5.3932203	-0.1920441	5.2481312
H	4.5982690	4.2938960	11.7661912
H	3.1171262	5.9414549	12.9387333
H	0.9029014	6.5849721	11.9840265
H	0.1182613	5.5082000	9.8416678
H	0.3927036	3.9389699	8.1020841
H	1.0350514	1.3083784	6.7711655
H	0.5546668	2.9380888	6.1793268
H	2.8560350	3.1137605	5.0592947
H	1.9873576	1.6510520	4.4796303
H	2.9903229	-2.0637306	10.0276135
H	4.9810924	-3.2727234	10.9328669
H	7.2894365	-2.3406105	10.6650071

H	7.6306200	-0.1510052	9.3934055
H	5.2981022	1.9702327	4.9754779
H	4.1894317	1.0382475	3.9284435
H	5.8167869	-0.1520257	6.2683900
H	6.2420343	-0.2951849	4.5386640
H	3.1232670	0.3711283	6.1383665
H	4.1545472	-1.5454571	4.3543919