Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Predictions of structures and properties of 2,4,6-triamino-1,3,5-triazine-1,3,5-trioxide (MTO) and 2,4,6-trinitro-1,3,5-triazine-1,3,5-trioxide (MTO3N) green energetic materials from DFT and ReaxFF molecular modeling

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We present the cell size information and xyz coordinates of the atoms for the most stable crystal structures of MTO and MTO3N obtained from cell optimization using periodic DFT calculations (PBE-ulg and PBE-D2).

1) MTO crystals

a) PBE-ulg

36
P21, a=4.5919, b= 6.9724,c= 10.0139, alpha= 90.0000, beta= 103.6406, gamma= 90.0000
C 0.258585 6.964800 6.128380
C 1.971728 3.478530 3.603069
C -1.445291 5.967120 7.463729
C 3.675605 2.480919 2.267720
C -0.488872 1.057504 8.128193
C 2.719186 4.543704 1.603256
N 1.062488 6.909579 5.097138
N 1.167826 3.423379 4.634311
N 2.316763 4.941619 7.653882
N -0.086450 1.455419 2.077567
N -0.391880 2.071779 8.977553
N 2.622193 5.557979 0.753895
N -1.361977 0.030051 8.342772
N 3.592290 3.516251 1.388678
N 0.359413 0.991684 7.062600
N 1.870900 4.477884 2.668850
N -0.694636 6.000587 6.327583
N 2.924949 2.514387 3.403866
H 1.771217 0.681831 4.911073
H 0.459097 4.168031 4.820376
H 0.928085 6.196302 4.348011
H 1.302229 2.710102 5.383438
H 2.419459 4.215722 6.942708
H -0.189146 0.729522 2.788742
H 2.080825 4.641876 8.614765
H 0.149488 1.155675 1.116684
H 0.397307 2.701944 8.807351
H 1.832983 6.188075 0.924196
H -1.218267 2.402689 9.499160
H 3.448580 5.888889 0.232290
O 1.291146 1.933656 6.921104
O 0.939168 5.419856 2.810345
O -0.849461 5.022569 5.443870
O 3.079775 1.536368 4.287579
O -2.119143 0.020359 9.453713
O 4.349457 3.506559 0.277736

b) PBE-D2

36
P21, a= 4.5047, b= 6.9121, c= 9.9978, alpha= 90.0000, beta= 104.3649, gamma= 90.0000
C 0.156986 6.897792 6.097718
C 1.867295 3.441742 3.587503
C -1.575721 5.914684 7.410841
C 3.600002 2.458634 2.274381
C -0.598549 1.054925 8.093262
C 2.622831 4.510975 1.591960
N 0.971120 6.835237 5.075250
N 1.053136 3.379187 4.610069
N 2.078577 4.903167 7.596603
N -0.054296 1.447117 2.088618
N -0.510194 2.063884 8.948564
N 2.534451 5.519934 0.736755
N -1.487561 0.036427 8.292583
N 3.511842 3.492477 1.392638
N 0.261243 0.982071 7.036217
N 1.763038 4.438121 2.649005
N -0.810979 5.943300 6.283093
N 2.835261 2.487250 3.402128
H 1.685214 0.667018 4.893167
H 0.339068 4.123067 4.792054
H 0.828842 6.127991 4.319512
H 1.195439 2.671941 5.365709
H 2.161633 4.166544 6.893069
H -0.137352 0.710495 2.792152
H 1.846934 4.608781 8.561252
H 0.177348 1.152731 1.123970
H 0.293272 2.688116 8.821010
H 1.731009 6.144166 0.864212
H -1.341405 2.386541 9.469048
H 3.365687 5.842590 0.216174
O 1.205010 1.914513 6.903820
O 0.819271 5.370563 2.781402
O -0.968022 4.974707 5.390116
O 2.992303 1.518658 4.295105
O -2.265181 0.043270 9.389532
O 4.289463 3.499320 0.295690

2) MTO3N crystals

a) PBE-ulg

72
P21/C, a= 11.4519, b= 9.0169, c= 8.4758, alpha= 90.0000, beta= 83.8774, gamma= 90.0000
C 3.062280 8.356592 2.681531
C 9.490843 0.660308 2.288409
C 6.057955 3.848142 4.773378
C 6.495168 5.168848 0.196561
C 1.049446 0.604222 2.647139
C 11.503677 8.412678 2.322800
C 8.070789 5.112672 4.807770
C 4.482334 3.904228 0.162169
C 1.170379 7.510987 1.605986
C 11.382744 1.505912 3.363953
C 14.815632 3.002537 0.878983
C -2.262509 6.014363 4.090956
N 4.491249 8.257857 2.964121
N 8.061874 0.759043 2.005818
N 4.628986 3.749407 4.490788
N 7.924137 5.267493 0.479152
N 0.240791 1.724121 3.116251
N 12.312332 7.292779 1.853688
N 8.879444 6.232571 4.338657
N 3.673679 2.784328 0.631282
N 0.485693 6.403802 0.912829
N 12.067430 2.613097 4.057111
N 15.500318 1.895352 1.572141
N -2.947195 7.121548 3.397798
N 0.463243 8.650272 1.852048
N 12.089879 0.366627 3.117891
N 15.522767 4.141823 0.632922
N -2.969645 4.875077 4.337018
N 2.459976 7.333354 1.992697
N 10.093147 1.683636 2.977242
N 13.526035 2.824905 0.492272
N -0.972911 6.192086 4.477667
N 2.363391 0.463559 3.073858
N 10.189733 8.553341 1.896081
N 6.756844 4.972009 4.381051
N 5.796279 4.044891 0.588888
O 4.846768 8.447663 4.125944
O 7.706355 0.569237 0.843995
O 4.273467 3.939213 3.328965
O 8.279656 5.077687 1.640975
O 5.205591 8.002950 1.992995
O 7.347464 1.013950 2.976994
O 10.780352 3.494500 0.492024
O 1.772772 5.522400 4.477915
O -0.935556 1.463262 3.383435

O	13.488679	7.553638	1.586504
O	10.055791	5.971713	4.071474
O	2.497331	3.045187	0.898466
O	0.795913	2.820667	3.222708
O	11.757403	6.196233	1.747232
O	8.324516	7.329117	4.232202
O	4.228801	1.687783	0.737738
O	-0.037649	5.567485	1.644205
O	12.590773	3.449415	3.325734
O	16.023661	1.059035	0.840765
O	-3.470537	7.957865	4.129175
O	-6.352120	6.432476	4.657578
O	18.905243	2.584424	0.312361
O	15.472356	1.924026	2.797330
O	-2.919232	7.092874	2.172609
O	3.062974	6.253401	1.721090
O	9.490149	2.763499	3.248849
O	12.923037	1.744950	0.763880
O	-0.369914	7.271949	4.206059
O	2.922324	1.335042	3.785652
O	9.630800	7.681858	1.184287
O	6.197912	5.843493	3.669256
O	6.355212	3.173408	1.300683
O	-0.697671	8.761992	1.369516
O	13.250793	0.254998	3.600423
O	16.683681	4.253542	1.115453
O	-4.130559	4.763448	3.854486

b) PBE-D2

72
P21/C, a= 11.2408, b= 8.9167, c= 8.3575, alpha= 90.0000, beta= 84.5057, gamma= 90.0000
C 3.044603 8.268813 2.630007
C 9.387772 0.647887 2.233082
C 5.989310 3.810374 4.664626
C 6.443065 5.106238 0.198463
C 1.032783 0.624169 2.600050
C 11.399591 8.292531 2.263038
C 8.001129 5.082519 4.694582
C 4.431245 3.834181 0.168506
C 1.151148 7.434210 1.548845
C 11.281227 1.482491 3.314243
C 14.679689 2.975860 0.882699
C -2.247314 5.940841 3.980389
N 4.480048 8.173047 2.891155
N 7.952327 0.743653 1.971934
N 4.553865 3.714697 4.403478
N 7.878510 5.202003 0.459610
N 0.225813 1.742591 3.082079
N 12.206563 7.174110 1.781009
N 8.808101 6.200941 4.212553
N 3.624275 2.715759 0.650535
N 0.458814 6.322208 0.868693
N 11.973560 2.594492 3.994395
N 15.372023 1.863858 1.562851
N -2.939648 7.052843 3.300237
N 0.447309 8.576350 1.794188
N 11.985065 0.340350 3.068900
N 15.383527 4.118000 0.637356
N -2.951154 4.798700 4.225732
N 2.438824 7.248386 1.939108
N 9.993551 1.668315 2.923980
N 13.392014 2.790035 0.492436
N -0.959639 6.126665 4.370652
N 2.344119 0.470891 3.035296
N 10.088255 8.445809 1.827792
N 6.689793 4.929241 4.259336
N 5.742581 3.987459 0.603752
O 4.856588 8.363152 4.046138
O 7.575788 0.553549 0.816950
O 4.177325 3.904801 3.248494
O 8.255050 5.011899 1.614594
O 5.178329 7.921062 1.908081
O 7.254046 0.995639 2.955007
O 10.652509 3.462711 0.523463
O 1.779866 5.453989 4.339625
O -0.955962 1.489000 3.331750
O 13.388337 7.427611 1.531338
O 9.989875 5.947439 3.962882

O	2.442500	2.969350	0.900206
O	0.786469	2.833103	3.219024
O	11.645906	6.083597	1.644064
O	8.247444	7.291453	4.075608
O	4.184932	1.625247	0.787480
O	-0.058768	5.493669	1.612551
O	12.491142	3.423032	3.250537
O	15.889605	1.035318	0.818993
O	-3.457230	7.881382	4.044096
O	12.909040	6.338258	4.506770
O	-0.476666	2.578442	0.356318
O	-3.875129	1.879908	2.787863
O	16.307503	7.036793	2.075226
O	3.037149	6.166344	1.667310
O	9.395227	2.750356	3.195778
O	12.793690	1.707994	0.764234
O	-0.361313	7.208706	4.098854
O	2.901282	1.329391	3.764419
O	9.531093	7.587309	1.098669
O	6.132630	5.787741	3.530213
O	6.299744	3.128959	1.332875
O	-0.711613	8.690038	1.307539
O	13.143987	0.226663	3.555550
O	16.542450	4.231688	1.124006
O	-4.110075	4.685013	3.739083