
Supporting Information

First-principles study of mechanical and optical behavior of plutonium oxide under typical structural phases and vacancy defects

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Table S1. Energies of AFM, FM and NM for β -Pu₂O₃, α -Pu₂O₃, γ -Pu₂O₃, PuO, α -PuO₂, γ -PuO₂.

Plutonium oxide	AFM energy(eV)	FM energy(eV)	NM energy(eV)
β -Pu ₂ O ₃	-57.565	-57.803	-53.971
α -Pu ₂ O ₃	-114.427	-115.147	-106.712
γ -Pu ₂ O ₃	-56.971	-57.476	-53.661
PuO	-95.555	-95.326	-88.435
α -PuO ₂	-133.580	-134.194	-122.877
γ -PuO ₂	-66.202	-66.560	-66.373

Crystal Coordinate Lists:

1. β -Pu₂O₃

Beta-Pu2 O3

1.0000000000000000

3.8821335015818668 -0.0000000000000000 -0.0000000000000000

-1.9410667507909334 3.3620262332915520 0.0000000000000000

-0.0000000000000000 -0.0000000000000000 5.8473959514856864

Pu O

2 3

Direct

0.3333333429999996 0.6666666870000029 0.2392150939910920

0.6666666870000029 0.3333333429999996 0.7607849200089091

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.3333333429999996 0.6666666870000029 0.6469546544250036

0.6666666870000029 0.3333333429999996 0.3530453155749937

2. α -Pu₂O₃

Alpha-Pu4 O6

1.0000000000000000

5.4591667217853903	0.0000000000000000	-0.0000000000000000
-0.0000000000000000	5.4591667217853903	-0.0000000000000000
0.0000000000000000	0.0000000000000000	5.4591667217853903

Pu O

4 6

Direct

0.7500000000000000	0.7500000000000000	0.2500000000000000
0.2500000000000000	0.7500000000000000	0.7500000000000000
0.7500000000000000	0.2500000000000000	0.7500000000000000
0.2500000000000000	0.2500000000000000	0.2500000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
-0.0000000000000000	-0.0000000000000000	0.5000000000000000
0.5000000000000000	0.0000000000000000	0.5000000000000000
0.0000000000000000	0.5000000000000000	0.5000000000000000
-0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000

3. γ -Pu₂O₃

Gamma-Pu2 O3

1.0000000000000000

3.8128837783244780	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.8128837783244780	0.0000000000000000
0.0000000000000000	0.0000000000000000	5.4622533667408222

Pu O

2 3

Direct

0.5000000000000000	-0.0000000000000000	0.7656124900952080
-0.0000000000000000	0.5000000000000000	0.2343874799047897
-0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	-0.0000000000000000
-0.0000000000000000	0.0000000000000000	0.5000000000000000

4. PuO

Pu4 O4

1.0000000000000000

5.1000370814982325	0.0000000000000000	-0.0000000000000000
-0.0000000000000000	5.1000370814982325	-0.0000000000000000
0.0000000000000000	-0.0000000000000000	5.1000370814982325

Pu O

4 4

Direct

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

5. α -PuO₂

Alpha-Pu4 O8

1.0000000000000000

5.4423906392051418	0.0000000000000000	-0.0000000000000000
0.0000000000000000	5.4423906392051418	0.0000000000000000
-0.0000000000000000	0.0000000000000000	5.4423906392051418

Pu O

4 8

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
0.2500000000000000	0.2500000000000000	0.7500000000000000
0.2500000000000000	0.7500000000000000	0.7500000000000000
0.2500000000000000	0.7500000000000000	0.2500000000000000
0.2500000000000000	0.2500000000000000	0.2500000000000000
0.7500000000000000	0.2500000000000000	0.2500000000000000
0.7500000000000000	0.7500000000000000	0.2500000000000000
0.7500000000000000	0.7500000000000000	0.7500000000000000
0.7500000000000000	0.2500000000000000	0.7500000000000000

6. γ -PuO₂

Gamma-Pu2 O4

1.0000000000000000

5.0696852698140988	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0696852698140988	0.0000000000000000
0.0000000000000000	0.0000000000000000	3.5456764326349082

Pu O

2 4

Direct

0.5000000000000000	0.5000000000000000	-0.0000000000000000
0.0000000000000000	0.0000000000000000	0.5000000000000000
0.8106049711684941	0.8106049711684941	-0.0000000000000000
0.1893950138315082	0.1893950138315082	0.0000000000000000
0.3106050011684966	0.6893950288315059	0.5000000000000000
0.6893950288315059	0.3106050011684966	0.5000000000000000

7. β -Pu₁₆O₂₃

Beta-Pu16 O23

1.000000000000000

7.1758626404266215	0.0000000451123670	-0.0000000000000000
-3.5879321086188645	6.2144788854106379	-0.0000000000000000
-0.0000000000000001	0.0000000000000000	11.6250200270611277

Pu O

16 23

Direct

0.1666666719999981	0.3333333429999996	0.1181211672423131
0.1666666719999981	0.3333333429999996	0.6172712263064412
0.1666302434863120	0.8333151587419565	0.1182710862193360
0.1646512803791248	0.8323256772102655	0.6184605288179018
0.6666849012580485	0.3333697715136858	0.1182710862193360
0.6676743827897395	0.3353487346208656	0.6184605288179018
0.6666849012556434	0.8333151587443616	0.1182710862193360
0.6676743828311326	0.8323256771688726	0.6184605288179018
0.3333223971021258	0.1666776178978717	0.3825402788742450
0.3359068749331593	0.1640931400668384	0.8771727175439581
0.3333223970975540	0.6666447951996833	0.3825402788742450
0.3359068749238237	0.6718137508569866	0.8771727175439581
0.8333552648003215	0.1666776179024439	0.3825402788742450
0.8281863091430184	0.1640931400761741	0.8771727175439581
0.8333333730000021	0.6666666870000029	0.3904430732544931
0.8333333730000021	0.6666666870000029	0.9017610773262582
0.0068830695353564	0.0137661390686800	0.9993116966997139
0.0000296294369735	0.0000592588795829	0.5024912400280551
0.0068830695333237	0.4931169304666764	0.9993116966997139
0.0000296294426090	0.4999703705573910	0.5024912400280551
0.5000000000000000	0.0000000000000000	-0.0054983588374144
0.5000000000000000	0.0000000000000000	0.5056616817751977
0.4862338609313200	0.4931169304646436	0.9993116966997139
0.4999407411204174	0.4999703705630265	0.5024912400280551
0.1666666719999981	0.3333333429999996	0.3183736671736397
0.1666666719999981	0.3333333429999996	0.8170230838173305
0.1650763838033789	0.8325382289029001	0.3192498879029815
0.1369721414523165	0.8184861077130765	0.8092954057361971
0.6674618310971049	0.3349236311966187	0.3192498879029815
0.6815139522869285	0.3630278735476872	0.8092954057361971
0.6674618310995124	0.8325382289004924	0.3192498879029815
0.6815139522607664	0.8184861077392399	0.8092954057361971
0.3344489205743142	0.1655510944256834	0.1830976282071985
0.3341954303921517	0.1658045846078459	0.6815372557674932
0.3344489205740486	0.6688978421483734	0.1830976282071985

0.3341954303996595	0.6683908617918151	0.6815372557674932
0.8311022178516314	0.1655510944259490	0.1830976282071985
0.8316091982081898	0.1658045846003381	0.6815372557674932
0.8333333730000021	0.6666666870000029	0.1833116605504539

8. β -Pu₁₆O₂₂

Beta-Pu16 O22

1.0000000000000000

7.1260304100758693	0.0000000512925963	-0.0000000000000000
-3.5630159823449219	6.1713229144091688	0.0000000000000001
0.0000000000000000	0.0000000000000001	11.6232405387481847

Pu O

16 22

Direct

0.1666666719999981	0.3333333429999996	0.1176294735541783
0.1666666719999981	0.3333333429999996	0.6176294665541814
0.1627943617019736	0.8313972178690093	0.1189146884978388
0.1627943617019736	0.8313972178690093	0.6189146814978415
0.6686028421309956	0.3372056532980173	0.1189146884978388
0.6686028421309956	0.3372056532980173	0.6189146814978415
0.6686028421670347	0.8313972178329775	0.1189146884978388
0.6686028421670347	0.8313972178329775	0.6189146814978415
0.3364093043696105	0.1635907106303882	0.3786246707916261
0.3364093043696105	0.1635907106303882	0.8786246707916261
0.3364093043463470	0.6728186097159600	0.3786246707916261
0.3364093043463470	0.6728186097159600	0.8786246707916261
0.8271814502840439	0.1635907106536508	0.3786246707916261
0.8271814502840439	0.1635907106536508	0.8786246707916261
0.8333333730000021	0.6666666870000029	0.4101755083050965
0.8333333730000021	0.6666666870000029	0.9101755083050966
0.0074492805972532	0.0148985612038494	0.0014168149243278
0.0074492805972532	0.0148985612038494	0.5014168149243279
0.0074492806065965	0.4925507193934041	0.0014168149243278
0.0074492806065965	0.4925507193934041	0.5014168149243279
0.5000000000000000	-0.0000000000000000	-0.0002798694351671
0.5000000000000000	-0.0000000000000000	0.4997201305648327
0.4851014387961500	0.4925507194027468	0.0014168149243278
0.4851014387961500	0.4925507194027468	0.5014168149243279
0.1666666719999981	0.3333333429999996	0.3176738927273645
0.1666666719999981	0.3333333429999996	0.8176738927273647
0.1338445745558428	0.8169223242736049	0.3102336294183179
0.1338445745558428	0.8169223242736049	0.8102336294183180
0.6830777357264001	0.3661554404441519	0.3102336294183179
0.6830777357264001	0.3661554404441519	0.8102336294183180
0.6830777357177608	0.8169223242822470	0.3102336294183179

0.6830777357177608	0.8169223242822470	0.8102336294183180
0.3355129891933669	0.1644870258066310	0.1826610183173968
0.3355129891933669	0.1644870258066310	0.6826610333173946
0.3355129891977238	0.6710259793910868	0.1826610183173968
0.3355129891977238	0.6710259793910868	0.6826610333173946
0.8289740806089181	0.1644870258022741	0.1826610183173968
0.8289740806089181	0.1644870258022741	0.6826610333173946

9. β -Pu₁₆O₂₀

Beta-Pu16 O20

1.0000000000000000

7.0098730056175818	-0.0064061483531669	0.0036648264263567
-3.5104851977894831	6.0803369881608234	-0.0000000005576083
0.0047771540781246	0.0027580912295320	11.6819367286318965

Pu O

16 20

Direct

0.1592354559608737	0.3296177349943026	0.1195273080919397
0.1592354559608737	0.3296177349943026	0.6195273010919428
0.1592354559608737	0.8296177649943055	0.1195273080919397
0.1592354559608737	0.8296177649943055	0.6195273010919428
0.6793526270973417	0.3396763130346965	0.1193231020061895
0.6793526270973417	0.3396763130346965	0.6193230950061926
0.6793526270973417	0.8396763430346986	0.1193231020061895
0.6793526270973417	0.8396763430346986	0.6193230950061926
0.3348905643978078	0.1674452826931959	0.3757348427631041
0.3348905643978078	0.1674452826931959	0.8757348427631041
0.3348905643978078	0.6674452976932007	0.3757348427631041
0.3348905643978078	0.6674452976932007	0.8757348427631041
0.8224783437697910	0.1612391573907815	0.4073485186548398
0.8224783437697910	0.1612391573907815	0.9073485186548399
0.8224783437697910	0.6612391723907862	0.4073485186548398
0.8224783437697910	0.6612391723907862	0.9073485186548399
0.0168841567211484	0.0084420783561872	0.0012576240548242
0.0168841567211484	0.0084420783561872	0.5012576240548240
0.0168841567211484	0.5084420783561870	0.0012576240548242
0.0168841567211484	0.5084420783561870	0.5012576240548240
0.4764100516626502	-0.0117949741639153	0.0006215469848563
0.4764100516626502	-0.0117949741639153	0.5006215469848567
0.4764100516626502	0.4882050258360844	0.0006215469848563
0.4764100516626502	0.4882050258360844	0.5006215469848567
0.1323573518245924	0.3161786829194566	0.3102353032603719
0.1323573518245924	0.3161786829194565	0.8102353032603720
0.1323573518245924	0.8161787129194592	0.3102353032603719
0.1323573518245924	0.8161787129194592	0.8102353032603720

0.7036736750183923	0.3518368369994740	0.3045168434729929
0.7036736750183923	0.3518368369994740	0.8045168434729931
0.7036736750183923	0.8518368669994766	0.3045168434729929
0.7036736750183923	0.8518368669994766	0.8045168434729931
0.3413845505474065	0.1706922757758139	0.1821863977108768
0.3413845505474065	0.1706922757758139	0.6821864127108745
0.3413845505474065	0.6706922907758187	0.1821863977108768
0.3413845505474065	0.6706922907758187	0.6821864127108745

10. β -Pu₁₆O₁₈

Beta-Pu16 O18

1.0000000000000000

6.9172239034526770	0.0000000787835836	0.0000000000000000
-3.4586126811472209	5.9904912028527422	-0.0000000000000000
-0.0000000000000000	-0.0000000000000000	11.7021015138445410

Pu O

16 18

Direct

0.1626335323346142	0.3373664826653839	0.1192754192901326
0.1626335323346142	0.3373664826653839	0.6192754122901358
0.1626335323517062	0.8252670936863259	0.1192754192901326
0.1626335323517062	0.8252670936863259	0.6192754122901358
0.6747329663136785	0.3373664826482913	0.1192754192901326
0.6747329663136785	0.3373664826482913	0.6192754122901358
0.6666666870000029	0.8333333730000021	0.1184415931183013
0.6666666870000029	0.8333333730000021	0.6184415861183044
0.3333333429999996	0.1666666719999981	0.3741997627496674
0.3333333429999996	0.1666666719999981	0.8741997627496675
0.3390540844468474	0.6695270577170092	0.4009582948104927
0.3390540844468474	0.6695270577170092	0.9009582948104927
0.8304730022829958	0.1609459305531510	0.4009582948104927
0.8304730022829958	0.1609459305531510	0.9009582948104927
0.8304730022701603	0.6695270577298440	0.4009582948104927
0.8304730022701603	0.6695270577298440	0.9009582948104927
0.0162931029689371	0.0081465514782358	0.0030792537590917
0.0162931029689371	0.0081465514782358	0.5030792537590917
-0.0000000000000000	0.5000000000000000	0.0011729506557776
-0.0000000000000000	0.5000000000000000	0.5011729506557777
0.4918534485092917	0.0081465514907071	0.0030792537590917
0.4918534485092917	0.0081465514907071	0.5030792537590917
0.4918534485217641	0.4837068970310640	0.0030792537590917
0.4918534485217641	0.4837068970310640	0.5030792537590917
0.1497205337047119	0.3502794812952837	0.3046181899391343
0.1497205337047119	0.3502794812952837	0.8046181899391341
0.1497205337217261	0.7994410964264461	0.3046181899391343

0.1497205337217261	0.7994410964264461	0.8046181899391341
0.7005589635735608	0.3502794812782715	0.3046181899391343
0.7005589635735608	0.3502794812782715	0.8046181899391341
0.6666666870000029	0.8333333730000021	0.3004030491210535
0.6666666870000029	0.8333333730000021	0.8004030491210534
0.3333333429999996	0.1666666719999981	0.1842436479586338
0.3333333429999996	0.1666666719999981	0.6842436629586315