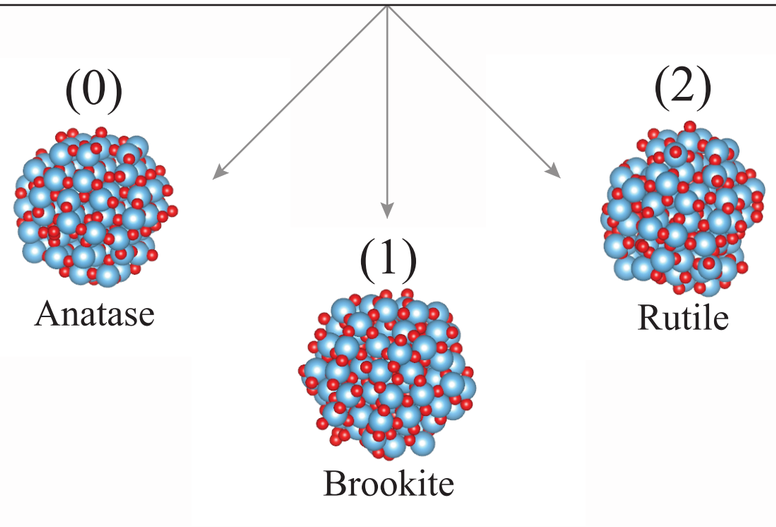
TDCM25

TASKS

Phase Classification



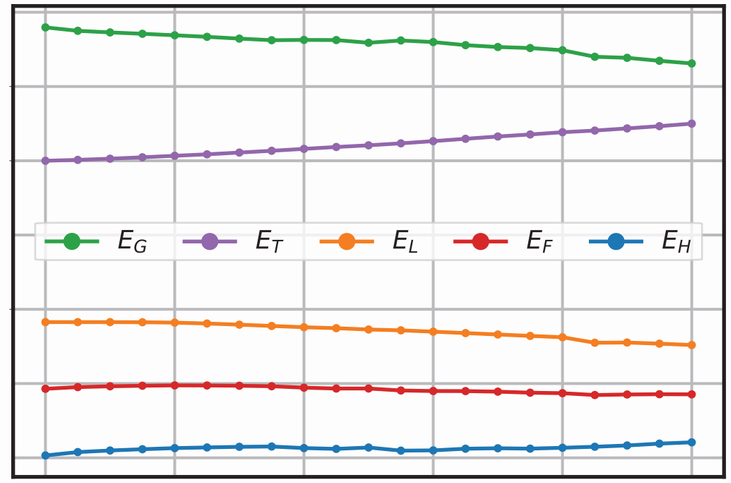
Explainability

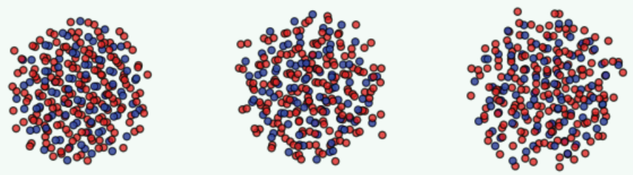
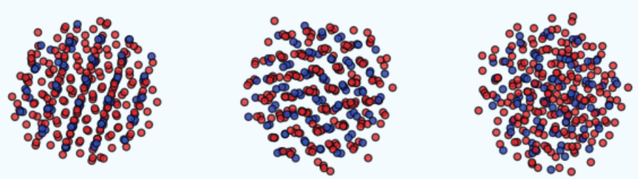
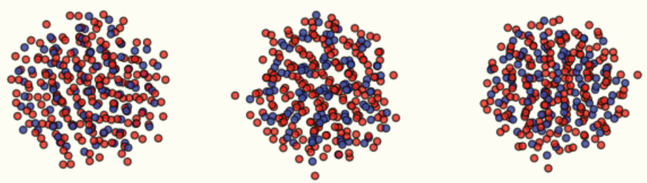
This anatase configuration at 300K consists of 223 atoms, including 96 titanium atoms and 127 oxygen atoms, resulting in a Ti:O ratio of approximately 0.76:1. The nanoparticle spans about 16.0 Å in x, 16.5 Å in y, and 16.0 Å in z. This is the original configuration (no rotation).

This is a brookite configuration at 500K consists of 100 atoms, including 50 titanium atoms and 50 oxygen atoms, resulting in a Ti:O ratio of approximately 1:1. The nanoparticle spans about 12.0 Å in x, 14.0 Å in y, and 10.0 Å in z. Rotation applied: x=30°, y=45°, z=60°.

This rutile configuration at 800K consists of 100 atoms, including 30 titanium atoms and 70 oxygen atoms, resulting in a Ti:O ratio of approximately 0.43:1. The nanoparticle spans about 43.0 Å in x, 45.0 Å in y, and 16.0 Å in z. Rotation applied: x=45°, y=30°, z=15°.

Property Prediction



Phase / Modality	Anatase	Brookite	Rutile
Text	This configuration at 0K consists of 268 atoms, including 88 titanium atoms and 180 oxygen atoms, resulting in a Ti:O ratio of approximately 0.49:1.The nanoparticle spans about 19.7 Å in x, 17.9 Å in y, and 18.5 Å in z. This is the original configuration (no rotation).	This configuration at 500K consists of 295 atoms, including 96 titanium atoms and 199 oxygen atoms, resulting in a Ti:O ratio of approximately 0.48:1. The nanoparticle spans about 17.6 Å in x, 17.8 Å in y, and 18.4 Å in z. Rotation applied: x=72.7°, y=-44.7°, z=-137.1°.	This configuration at 1000K consists of 287 atoms, including 89 titanium atoms and 198 oxygen atoms, resulting in a Ti:O ratio of approximately 0.45:1. The nanoparticle spans about 18.4 Å in x, 18.6 Å in y, and 17.8 Å in z. Rotation applied: x=58.9°, y=38.9°, z=-104.8°.
Image			
XYZ	X Ti 48.19832198 43.16842672 38.98264469 Ti 49.27877350 40.25000809 40.26030152 Ti 45.87885744 45.44320271 38.01740063 Ti 45.23448385 47.16625656 40.42685497 ... O 37.96192047 39.71976610 38.34647828 O 39.83005324 39.69168496 40.72952811 O 37.76759860 37.82759287 35.82859873 O 39.62493126 38.00156066 33.30703226	Y Ti -42.64310588 -74.34912331 -49.12931380 Ti -34.20277088 -70.17183774 -54.60438490 Ti -44.37017132 -69.68829779 -47.34065195 Ti -30.63534111 -67.62447133 -42.11489172 ... O -28.70818063 -66.00876419 -45.83320709 O -30.46921988 -63.45782988 -46.78879161 O -27.87845838 -68.50097564 -47.56092028 O -30.94393141 -65.98235914 -51.06262144	Z Ti -11.92292751 -33.72547796 41.71110621 Ti -6.133062460 -36.50977673 40.62169986 Ti -13.20554663 -35.47418294 39.53811896 Ti -14 84633316 -33.34047768 34 49905360 ... O -0.054868980 -33.93664624 33.91028883 O -15.16869459 -25.56954253 38.06331951 O -8.259863160 -38.02779467 37.53792462 O -12.95029921 -37.28066736 39.79491854