Crystal Structure:

TiO2 (Rutile)

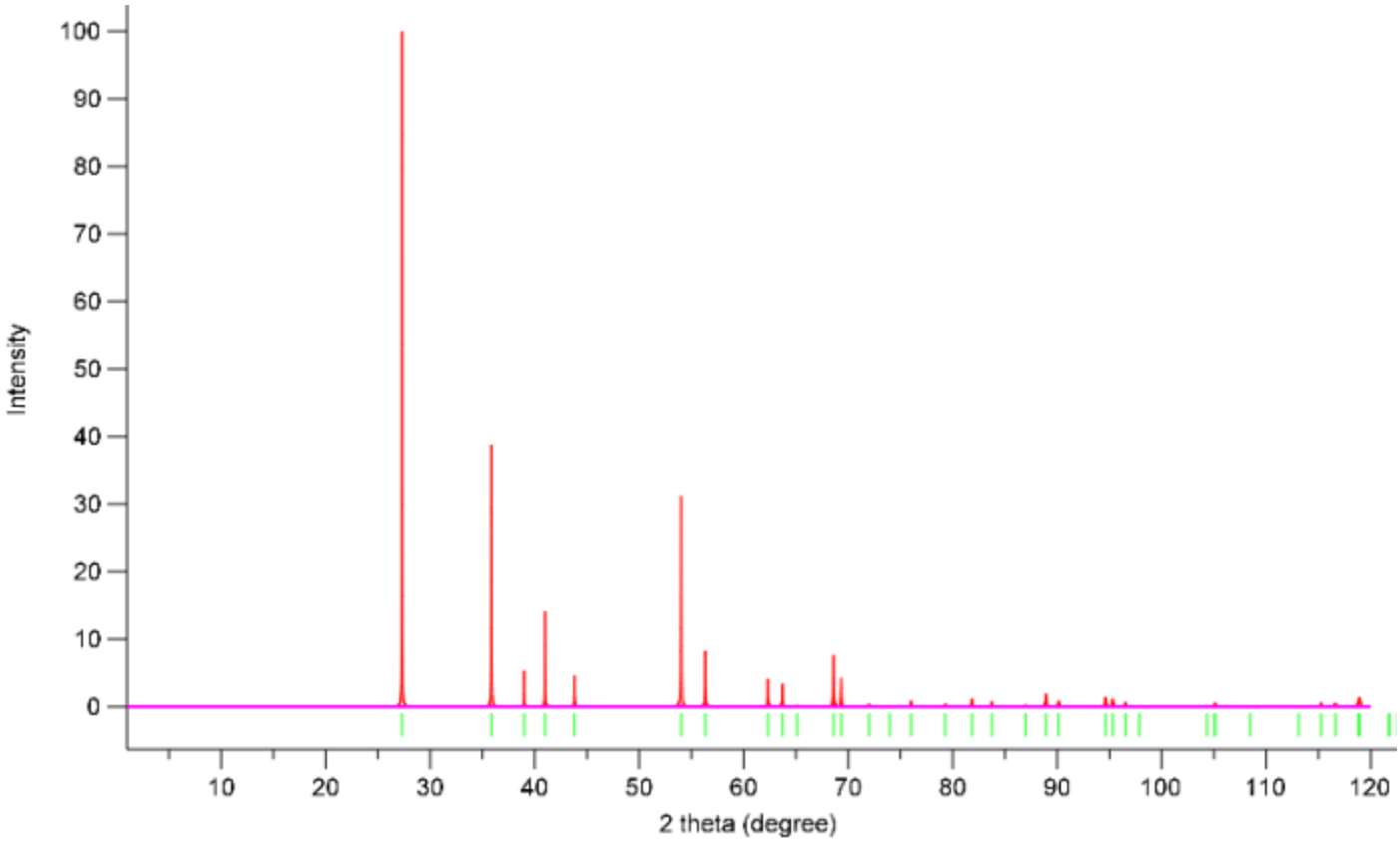
About/Help

CIF Source:
Meagher E P, Lager G A
The Canadian Mineralogist 17 (1979) 77-85
Polyhedral thermal expansion in the TiO2 polymorphs: Refinement
of the crystal structure of rutile and brookite at high temperature
Sample at 600 degrees C
_database_code_amcsd 0005166
4.616 4.616 2.977 90 90 90 P4_2/mnm

http://rruff.geo.arizona.edu/AMS/download.php?id=05870.cif&down=cif

Simulated Powder XRD using VESTA:

X-Ray Wavelength: 1.54059 Angstrom



Powder XRD pattern simulation of TiO2 (Rutile)

Simulation 1: GGA

Pseudopotential Used:
Ti.pbe-spn-kjpaw_psl.1.0.0.UPF
O.pbe-n-kjpaw_psl.1.0.0.UPF

PP Type: Ultrasoft
Exchange Correlation Functional: PBE-GGA

Non-linear core corrections are used.

Wavefunction Energy Cutoff: 51 Ry
Charge Density Energy Cutoff: 561 Ry
k – mesh: 8x8x8
Run Type: GGA-PBE

Total Energy vs Cutoff:

Cutoff(Ry)	Total Energy(Ry)
30	-534.25360543
35	-534.68616320
40	-534.78130295
45	-534.80017080
50	-534.80392479
51	-534.80436774
53	-534.80522769
55	-534.80611408

Optimized Coordinates and Lattice Parameters:

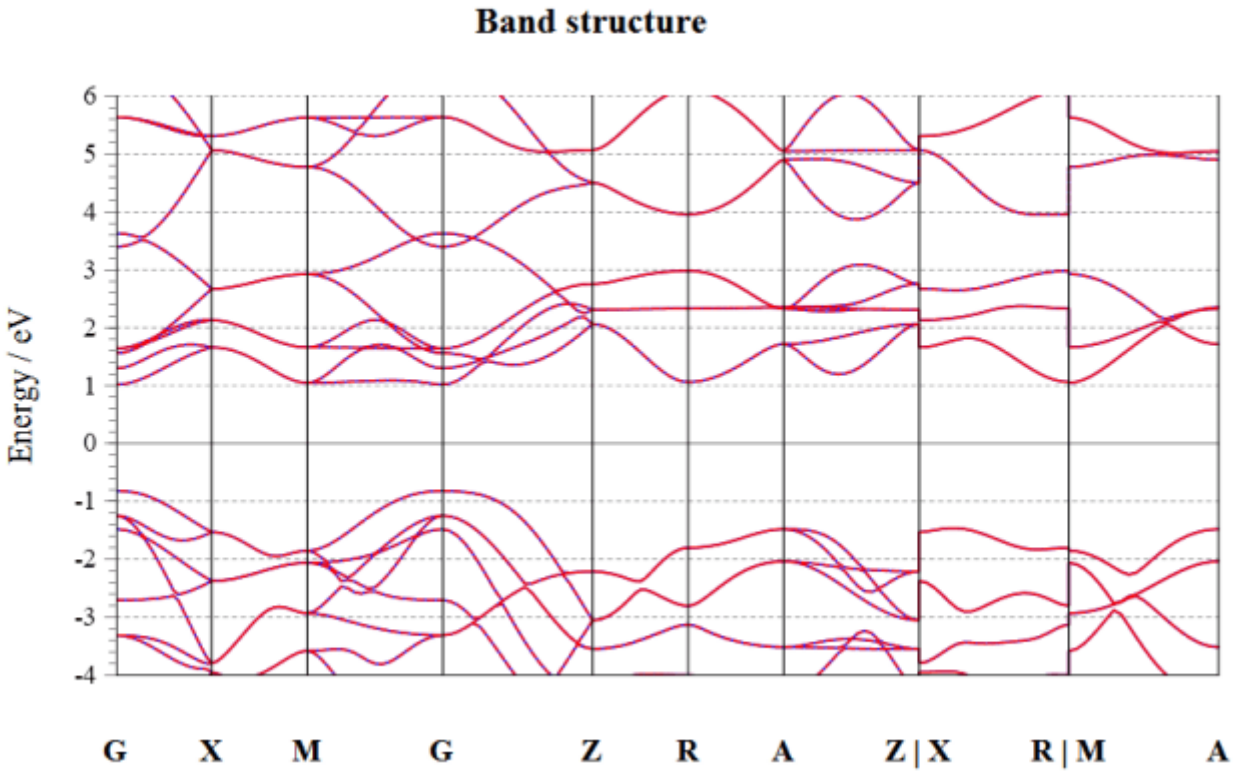
CELL_PARAMETERS {angstrom}

4.644336	-0.000037	0.000000
-0.000037	4.644336	0.000000
0.000000	0.000000	2.969167

ATOMIC_POSITIONS {angstrom}

Ti	0.000000	0.000000	0.000000
Ti	2.3221	50 2.322150	1.484584
O	1.416216	1.416216	0.000000
O	3.228083	3.228083	0.000000
O	3.738386	0.905913	1.484584
O	0.905913	3.738386	1.484584

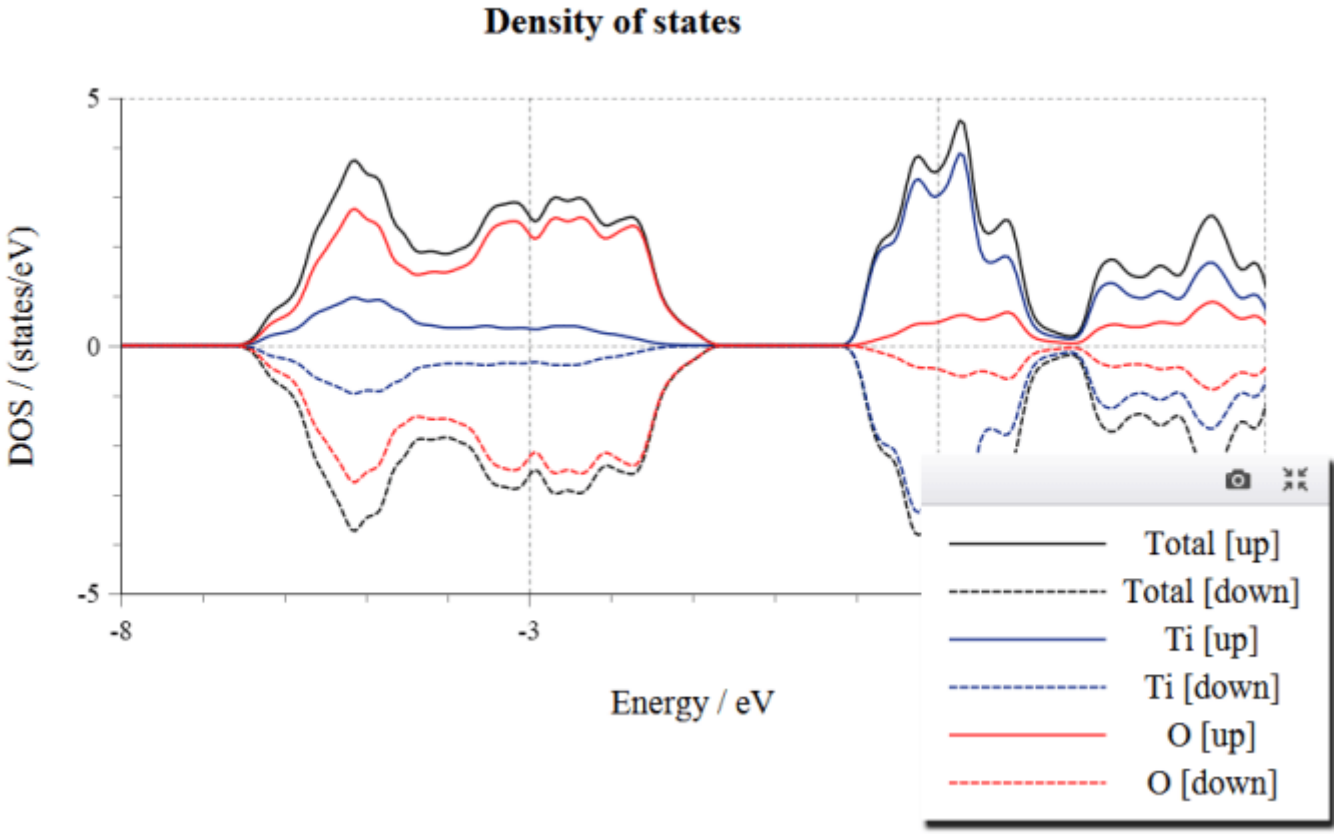
Bandstructure:



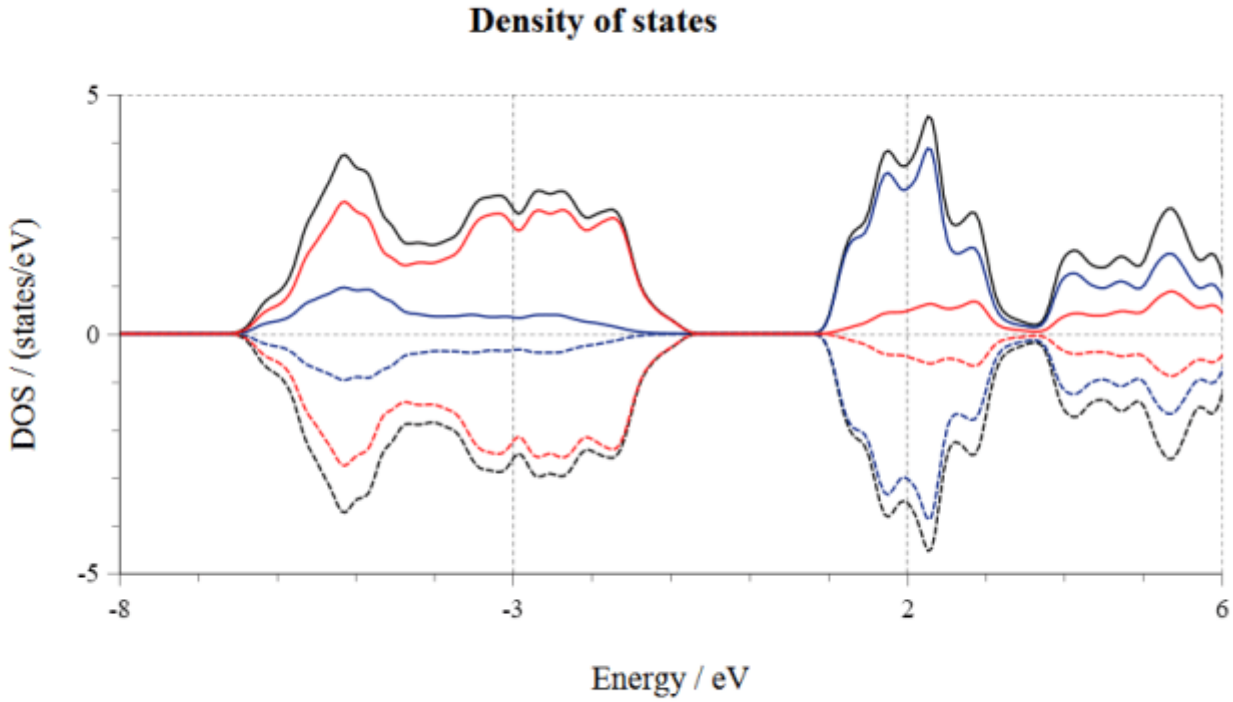
Bandstructure along high-symmetry points of TiO2 (Rutile)

Band-gap: 1.8 eV (approx.)

Density of States(DOS):



Total and Projected Density of States of TiO2 (Rutile)



Input Files:

Acknowledgements:

I acknowledge the use of the following tools and packages in order to produce the above simulations.
Quantum Espresso(for DFT based simulations): http://www.quantum-espresso.org/
BURAI(for visualization and as a GUI for QE): http://nisihara.wixsite.com/burai
VESTA(for visualization and XRD simulations): http://jp-minerals.org/vesta/en/

References and Resources

https://en.wikipedia.org/wiki/Rutile

https://www.researchgate.net/publication/51554133_DFT_U_Calculations_of_Crystal_Lattice_Electronic_Structure_and_Phase_Stability_under_Pressure_of_TiO2_Polymorphs

https://www.sciencedirect.com/science/article/pii/S0022369716300452

Manas Sharma
I'm a physicist specializing in theoretical, computational and experimental condensed matter physics. I like to develop Physics related apps and softwares from time to time. Can code in most of the popular languages. Like to share my knowledge in Physics and applications using this Blog and a YouTube channel.

Share this:

Like this: