Crystal Structure:

TiO2 Anatase

CIF Source:
Acta Crystallographica B47 (1991) 462-468
Structural and thermal parameters for rutile and anatase
Locality: synthetic
_database_code_amcsd 0019093
http://rruff.geo.arizona.edu/AMS/CIF_text_files/11272_cif.txt

Simulated Powder XRD using VESTA:

X-Ray Wavelength: 1.54059 Angstrom

Simulation 1: GGA

Pseudopotential Used:
Ti.pbe-spn-rrkjus_psl.1.0.0.UPF
O.pbe-nl-rrkjus_psl.1.0.0.UPF

PP Type: Ultrasoft
Exchange Correlation Functional: PBE-GGA
Non-linear core corrections are used.

Total Energy vs Cutoff:
E-Cutoff(Ry) Total E(Ry)
Wavefunction Energy Cutoff: 54 Ry
Charge Density Energy Cutoff: 600 Ry
k - mesh: 8x8x8
Run Type: GGA-PBE

Optimized Coordinates and Lattice Parameters:

Lattice Parameters: a = b = 3.80034 Å, c = 9.70793 Å
alpha = beta = gamma = 90 degrees
TiO$_2$ (Anatase) – DFT Study

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ATOMIC_POSITIONS {angstrom}
Ti 0.000000  0.000000  0.000000
Ti 1.900170 1.900170  4.853964
Ti 0.000000  1.900170  2.426988
Ti 1.900170  0.000000  7.280940
O 0.000000  0.000000  2.005006
O 1.900170  1.900170  6.858963
O 0.000000  1.900170  4.431988
O 1.900170  0.000000  9.285942
O 1.900170  1.900170  2.848965
O 0.000000  0.000000  7.702922
O 1.900170  0.000000  5.275940
O 0.000000  1.900170  0.421986

Bandstructure:

Bandstructure of TiO$_2$ (Anatase) simulated using Quantum Espresso

High Symmetry points: G-X-M-G-Z-R-A-Z (Brillouin Zone integration along these points)

Density of States(DOS):
TiO$_2$ (Anatase) – DFT Study

**Input Files:**

TiO$_2$ Anatase Input Files
Simulation 2: GGA + U(Hubbard Correction)

The Hubbard parameter provides on-site Coulomb corrections to the highly localized electrons. It can usually be determined by the linear response approach.

Variation of Band Gap with Hubbard Parameter U:

using simplified version of Cococcioni and de Gironcoli, PRB 71, 035105 (2005), using Hubbard_U

<table>
<thead>
<tr>
<th>U(eV)</th>
<th>Band-Gap(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.2182</td>
</tr>
<tr>
<td>2</td>
<td>2.2974</td>
</tr>
<tr>
<td>3</td>
<td>2.3862</td>
</tr>
<tr>
<td>4</td>
<td>2.4892</td>
</tr>
<tr>
<td>5</td>
<td>2.6094</td>
</tr>
<tr>
<td>6</td>
<td>2.7540</td>
</tr>
<tr>
<td>7</td>
<td>2.9287</td>
</tr>
<tr>
<td>8</td>
<td>3.1443</td>
</tr>
<tr>
<td>9</td>
<td>3.4117</td>
</tr>
</tbody>
</table>

Therefore, the rest of the calculations will be run using U=8eV:

(Note: Just because U=8eV provided a good picture of the band-gap doesn’t mean that it will provide a good...
Such a high correction can change other properties and therefore, the parameter should be suitably determined. For more info read the article attached in the References section of this article.

Bandstructure:

Density of States(DOS):
Input Files:

TiO2 Anatase 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:

Manas Sharma

PhD researcher at Friedrich-Schiller University Jena, Germany. 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.

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