From Atoms to Materials: Predictive Theory and Simulations

Week 1 – Homework solution 3

Nicolas Onofrio, David guzman and Alejandro Strachan
nonofrio@purdue.edu
School of Materials Engineering
Purdue University
West Lafayette, Indiana USA
Electronic structure of Oxygen atom

- DFT calculation with SeqQuest tool on nanohub
- Electronic configuration of O: $1s^22s^22p^4$

This tutorial explains how to compute the energy of these two spin states.
Electronic structure of Oxygen atom

- DFT calculation with SeqQuest tool on nanohub

From your dashboard search for SeqQuest.
Electronic structure of Oxygen atom
Electronic structure of Oxygen atom

- Input parameters: Geometry

![Diagram of nanoMATERIALS SeqQuest DFT interface]

- Pre-built molecular systems
- Coordinate style
- Title for the simulation
- Input geometry
- Simulation box size
- Boundary conditions
Electronic structure of Oxygen atom

- **Input parameters: Geometry**

  I started here from O2 molecule and modified the input Cartesian coordinates. Title for the simulation: 1: total number of atoms. Oxygen atom: another title. 0 0.00 0.00 0.00: atom-type x y z. 3 vectors to define the box size. Molecule type calculation.
Electronic structure of Oxygen atom

- **Input parameters: Energy expression**

- **Functional used for the DFT calculation (GGA or GGA-SP)**
- **Numerical integration parameters**
- **Energy convergence criterion**
- **|Number spin up – number spin down|**
- **Charge of the system**

Here we keep all the default parameters and just specify the spin state (spin polarization).

In the case of the singlet state, $|\text{Number spin up} - \text{Number spin down}| = 4 - 4 = 0$ (see slide 1).

In the case of the triplet state, $|\text{Number spin up} - \text{Number spin down}| = 5 - 3 = 2$ (see slide 1).

Remember to select GGA-SP (spin polarized for the triplet state).
Electronic structure of Oxygen atom

Run the simulation

You can specify the geometry relaxation parameters and some advanced parameters. We keep all the defaults parameters.
### Electronic structure of Oxygen atom

**Binding energy =** 0.5405188827 Ry = 7.3542 eV

**AFTER ITERATIONS =** 0.00 = 3.0 seconds used ( 0.00 usr 0.00 sys)

atom x0000 stress term= 6.5454751140

total force contributions(Ry/bohr):

<table>
<thead>
<tr>
<th></th>
<th>x force</th>
<th>y force</th>
<th>z force</th>
</tr>
</thead>
<tbody>
<tr>
<td>atom</td>
<td>0.000000000</td>
<td>0.000000000</td>
<td>0.000000000</td>
</tr>
<tr>
<td>f-defect</td>
<td>0.000000000</td>
<td>0.000000000</td>
<td>0.000000000</td>
</tr>
</tbody>
</table>

**AFTER FORCE RTNS =** 0.45 = 3.5 seconds used ( 0.45 usr 0.00 sys)

xref, max force= 0.000000000 0.000000000 for component# 1

Final geometry for step 1 of 1 total
atom, type, position: step# 1

<table>
<thead>
<tr>
<th></th>
<th>x force</th>
<th>y force</th>
<th>z force</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000000000</td>
<td>0.000000000</td>
<td>0.000000000</td>
</tr>
</tbody>
</table>

Final relaxed energy = -31.5511731173

***** ERROR: gromdata/unknown input command
Total TIME used= 3.5 seconds (user= 3.5 sys= 0.0)

... wait a minute ...
Electronic structure of Oxygen atom

- **Output:** Analysis of the result

There are different ways to analyze the result.
Electronic structure of Oxygen atom

- Output: Analysis of the result

<table>
<thead>
<tr>
<th>Step</th>
<th>Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-31.5511731173</td>
</tr>
<tr>
<td>2</td>
<td>-31.5511731173</td>
</tr>
<tr>
<td>3</td>
<td>-31.5511731173</td>
</tr>
<tr>
<td>4</td>
<td>-31.5511731173</td>
</tr>
<tr>
<td>5</td>
<td>-31.5511731173</td>
</tr>
<tr>
<td>6</td>
<td>-31.5511731173</td>
</tr>
</tbody>
</table>

The data tab give us the final total energy of -31.5511731173 eV.