Online simulations via nanoHUB: Exchange interaction in Oxygen

In this tutorial:
• Setup DFT simulation for an oxygen atom
• Explore how the total spin affects total energy
• Quantify exchange energy

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STEP 1: launch the SeqQuest tool

From your My HUB page launch seqQuest

• From All Tools find: nanoMaterials SeqQuest DFT
• Launch tool by clicking on:
STEP 2: setup the atomistic simulation cell

From the *Input Geometry* tab of the tool

We will select the O2 molecule pre-build case and modify it.

Only 1 atom (1st line)
Oxygen atom at position
0.0, 0.0, 0.0 (3rd line)
Make sure there are no extra lines (even at the end) and do not use tabs.

Box for simulation (10 Angstroms on the side):
10.0  0.0  0.0
0.0  10.0  0.0
0.0  0.0  10.0

STEP 3: setup the spin state to be considered

Spin 1 configuration (triplet)
- Set GGA-SP (for exchange & correlation)
- Set spin polarization to 2 (this number is the difference between spin up and spin down electrons)

Spin 0 configuration (singlet)
- Set GGA
- Spin polarization to 0 (same number of spin up as down)
STEP 4: set type of run and simulate!

Calculation specification tab

We have a single atom so the atomic force will always be zero. No need to compute force or relax the atomic structure

Click simulate
And wait for the results (a minute or so)

STEP 5: analyze total energy

Select Data from the output pull-down menu

Total energy of the system is listed below “Total Converged Energy”

For the spin 1 case (the two unpaired electrons with same spin) the energy is -31.669 Ryd
STEP 5: Report

- What is the energy difference between the spin 1 and spin 0 states?

- How large is this compared to a bond energy or the electron binding energy in hydrogen?

- Explain the physics behind the energy difference