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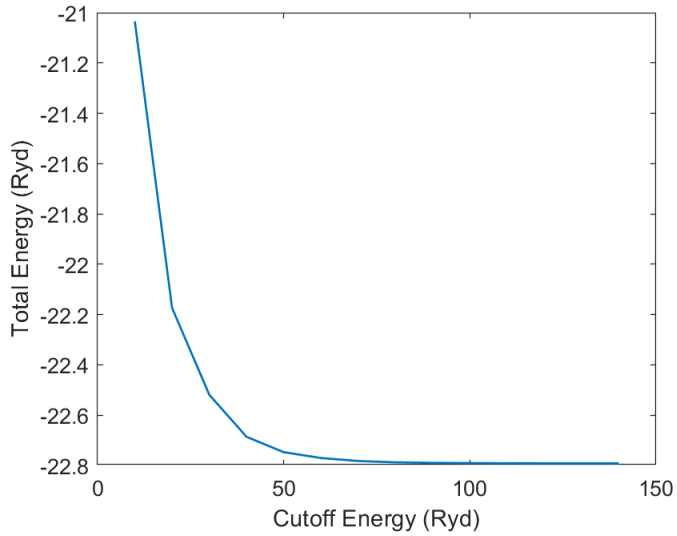
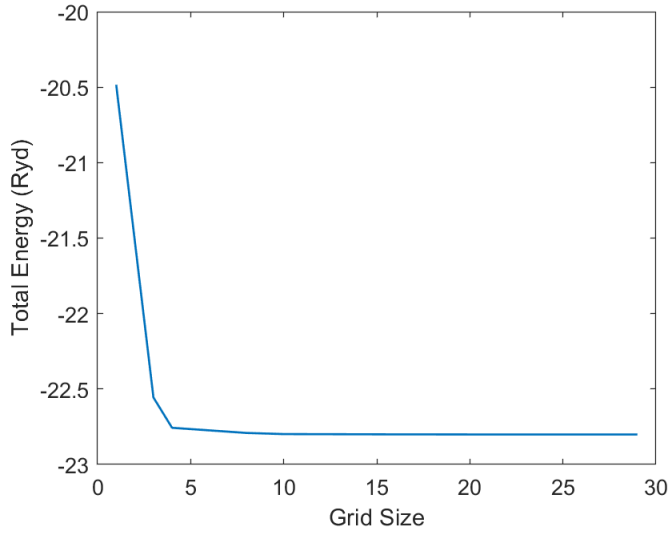
ME 556

QM Lab 2 - Quantum Espresso

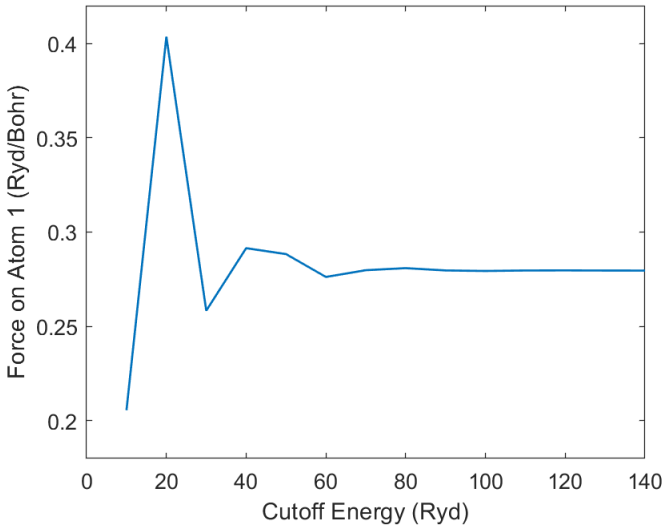
1. Total energy as a function of cutoff energy, which ranged from 10 to 140 Ryd by increments of 10 Ryd. The convergence value was calculated to be 110 Ryd. This means the change from 100 to 110 Ryd is less than 5 meV/atom. As cutoff energy increases towards infinity the total energy approaches some value asymptotically (about -22.79157949). The calculations with a primitive cell are more efficient than using the cubic cell, whereas calculations using the cubic cell could give more information.



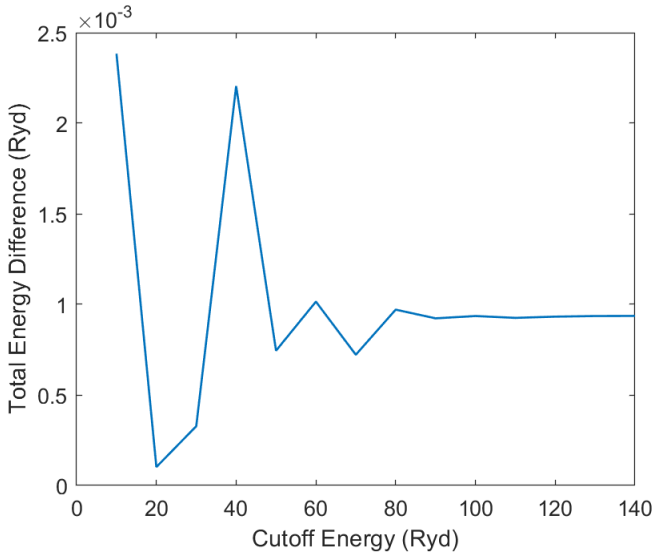
2. Total energy as a function of k-point grid size. The k values ranged from 1 to 8 by increments of 1, resulting in the grid sizes 1, 3, 4, 8, 10, 16, 20, and 29 respectively. Convergence was calculated to occur at a grid size of 20 using the same method as the previous problem. This results in the same trend as problem 1, converging towards an energy value as grid size increases.



3. A C atom was displaced by +0.05 in the z direction resulting in the plotted force on atom 1 as a function of the cutoff energy. The force on atom 2 is equal in magnitude but the opposite sign, for this reason only atom 1 is plotted. Convergence was calculated with the condition that a change in force of less than 10 meV/Angstrom signifies convergence. The cutoff energy value for convergence is 100 Ryd.

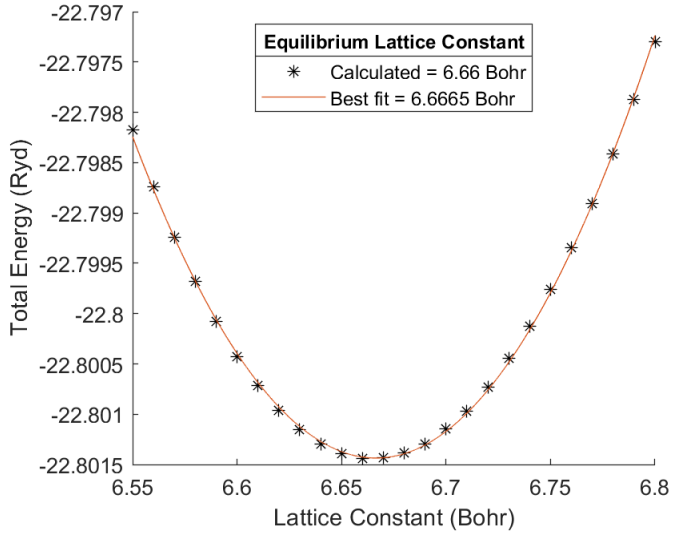


4. Total energies for both the lattice parameters of 6.74 and 6.70 Bohr were calculated with cutoff energies ranging from 10 to 140 Ryd by increments of 10 Ryd. Plotted below is the difference between these total energies for each lattice parameter versus the respective cutoff energy. The condition for convergence is a change less than 5 meV/atom. This first occurs at a cutoff energy of 30 Ryd, but larger changes occur at 40 and 50 Ryd. Thus the total energy is converged at a cutoff energy value of 60 because all subsequent changes are less than 5 meV/atom.

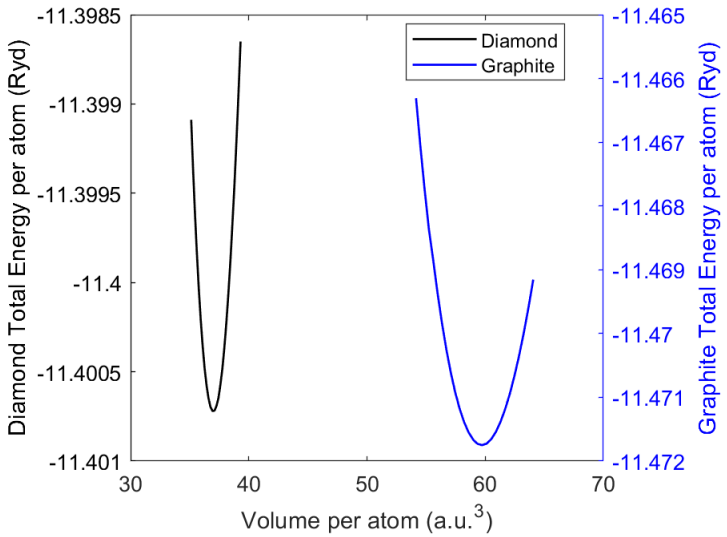


5. The 3 convergence values when looking at absolute energies, forces, and energy difference are 110 , 100, and 60 Ryd respectively. For problems 1 through 4 the number of k points at the converged values were 8, 20, 18, and 8 respectively. The converged cutoff energy values result in a higher amount of k points than lower cutoff energies. To ensure accurate QM calculations one would need to make sure each value converges individually and then use those values in that range for subsequent calculations. Use a sufficiently large number of k-points and a converged cutoff energy value.

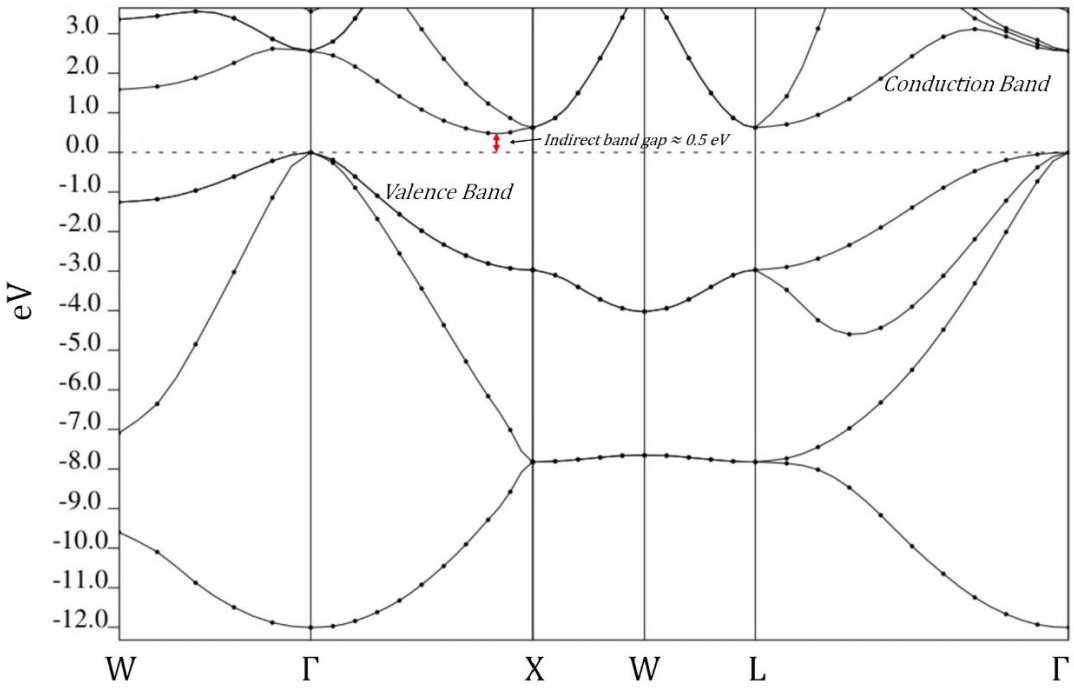
6. Equilibrium lattice of constant of diamond was found to be 6.66 Bohr by PWSCF calculation. The total energy for multiple lattice parameters was calculated and the one that resulted in the least total energy is the equilibrium lattice constant. The bulk modulus for diamond was calculated to be 206 GPa using the formulas provided in the instructions and the data obtained for this problem.



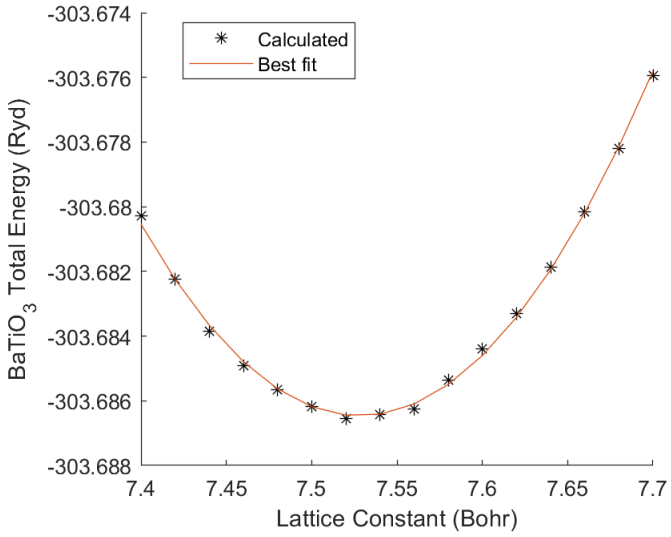
7. Below energy per atom for both diamond and graphite are plotted as a function of volume per atom. Here the diamond calculations contained 2 atoms per primitive cell while the graphite contained 4 atoms per primitive cell. The lattice constant of graphite was calculated to be 4.66 Bohr. This plot tells us that as pressure changes the equilibrium phase changes. For high pressure the equilibrium phase will be diamond.



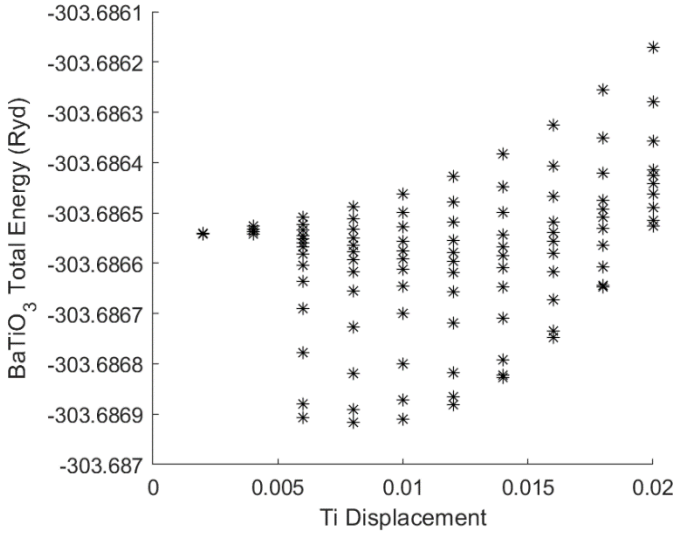
8. Silicon band structures are plotted below with the points of symmetry labeled. Silicon has a total of 4 valence electrons. The valence bands are seen below zero on the eV axis and the conduction bands are above zero on the eV axis. The indirect band gap looks to be about 0.5 eV, which is less than the 1.17 eV measured experimentally.



9. The lattice parameter for $BaTiO_3$ was determined to be 7.52 Bohr. This is the value with the lowest total energy for a cubic lattice. The minimum energy is -303.6865 Ryd.



Plotted below is the total energy as a function of Ti displacement along the cubic lattice. The minimum energy calculated here is -303.6869 Ryd. This results in an energy difference of 0.0004 Ryd with the minimum energy calculated on the previous plot.



Using the script to displace Ti and O the final energy was found to be 1943.387 Ryd and the final positions of the atoms are:

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ATOMIC_POSITIONS
Ba            0.0000000000        0.0000000000        0.0000000000
Ti            0.5000000000        0.5000000000        0.0744893156
O             0.5000000000        0.5000000000       -0.0664893617
O             0.5000000000        0.0000000000        0.5000000139
O             0.0000000000        0.5000000000        0.5000000139
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10. Quantum calculations can help to determine if a material is an insulator, conductor, or semiconductor through calculating the band structure and determining the band gap size. Also the minimum energy lattice constants can be calculated, which is directly related to the bulk modulus and other material properties. Finally, different phases of a material, diamond and graphite, both composed of carbon, can be compared which is helpful in determining how and why the phases form.