

Chem 3430
Assigned Oct. 11

HW #4
Due Oct.. 29

1. Consider a one-dimensional chain of Be atoms. Using the B3LYP/6-31G(d) method with 32 kpoints, calculate the optimal Be-Be spacing assuming all nearest neighbor Be-Be distances are the same.

Now check to see if this structure is unstable with respect to bond alternation. If so, what is the geometry and the energy lowering per atom?

How is the band structure changed by the introduction of bond alternation?

2. Do a calculation [B3LYP/6-31G(d) with 16 kpoints] on bulk Si using the experimental geometry and lattice constant. What do you get for the direct and indirect band gaps, and how does this compare with experiment?

Cleave the surface in the (100) direction. Form a surface dimer with the geometry from the literature. How is the electronic structure of the system with the surface different from that of the bulk?