Ch 121a HW

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1 Problem 1

1.1 Part a

ISMEAR determines how the partial occupancies are set for each orbital. It provides many options to choose from, of which we only used one.

1.2 Part b

SIGMA specifies the width of the smearing in eV. Its default is 0.2.

1.3 Part c

If you have no a priori knowledge of your system, for instance, if you do not know whether your system is an insulator, semiconductor or metal then always use Gaussian smearing ISMEAR=0 in combination with a small SIGMA=0.03-0.05.

2 Problem 2

2.1 Part a

The 4 Å box gives an electronic free energy of -15.457164 eV. The 15 Å box gives an electronic free energy of -14.767794 eV. The 4 Å box gives a lower energy, since the atoms are closer, thus there will be stronger vdW interactions.

2.2 Part b

Pure, dry air has a density of 1.293 kg/m^3 at a temperature of 273 K and a pressure of 101.325 kPa, according to NASA. The 4 Å box gives a density of 726.7622882763201 kg/m^3. This is 562.5 times denser than pure air, which is not realistic. The 15 Å box gives a density of 13.781566355462072 kg/m^3, which is more realistic.

3 Problem 3

Using the calculation results from carbon monoxide from 15 Å box, because this is more similar to the actual density of air.

3.1 Part a

2.44 eV

3.2 Part b

2.41 eV

3.3 Part c

0.92 eV

3.4 Part d

The top site binds CO the strongest