# 10.675 Assignment #4

due 10/21/04

In this problem set, you will use Car-Parrinello Molecular Dynamics (CPMD) to calculate the adsorption energy of oxygen atom on the Si(100) surface and compare it to the experimental data that you can find.

Solution:
This is really a trivial problem set. It has the objective of getting you familiar with CPMD calculations and familiar with using the NCSA supercomputer. The results are summarized in the following table.

| System | Energy (a.u.) |
|---|---|
| **Atomic O** | -14.64507328 |
| **Si (100)** | -46.34381829 |
| **O-Si(100)** | -61.20165854 |
| **AE /a.u.** | -0.21276697 |
| **AE /kcal/mol** | -133.5 |

From the results, we can see that the adsorption energy of oxygen atom on the Si(100) surface is about 133.5 kcal/mol, while the experimental value is about 165 kcal/mol [Surface Science **268** (1992) 238-264]. The difference between experiment and simulation could be caused by the following reasons:

a. ignoring surface relaxation
b. approximate functional
c. small planewave cutoff
d. finite temperate and pressure effects
e. experimental uncertainty