INSTRUCTIONS

Due date: Morning, Dec. 11, 2006

• Calculation on a clean surface (slab)

1. Make a POSCAR file for a slab of 2x2 unit cell.

2. Download the putty, winscp and raswin packages from the following website respectively:
   http://www.putty.nl/download.html
   http://winscp.net/eng/download.php
   http://www.bernstein-plus-sons.com/software/RasMol_2.7.2.1.1

3. Double click on putty icon and login to pemfc.

4. Run the following command to copy all the necessary input files into your home directory.
   ```
   cp   -r   /usr/local/pemfc/*   .
   ```
   (don’t forget the “.” At the end of the line)

5. Make a new folder for your slab calculations.

6. Change your current directory (see appendix C) to either INPUT_for_H_adsorption_on_Pd or INPUT_for_CO_adsorption_on_Pd directories (depending on your project) and copy the necessary input files (INCAR, POTCAR, KPOINTS) into the directory you have created in 4.

7. Double click on “winscp” icon and login to pemfc so that you will be able to transfer your POSCAR to your folder in pemfc cluster.

8. Transfer the POSCAR to pemfc by drag and drop to the folder you have made in 4. Now using “ls” in SSH shell (putty) you should be able to see input files and POSCAR file.

9. Do pdb to make a pdb format of your POSCAR. Call the output file POSCAR.pdb.

10. Transfer it to your local computer and view it using “raswin”.

11. If you see some defects in your POSCAR try to correct it and redo from 8.

12. Now you are ready to run the vasp program. See appendix A to find out how to run the program.

At the end of the program you will see the total energy of the slab and forces on each ion stored in OUTCAR. Look for the total energy in the last iteration at OSZICAR or OUTCAR. In addition, the file CONTCAR will provide you the final position of the ions. Make a pdb format of CONTCAR file. Then transfer the pdb file to your local computer and view it by raswin and obtain the relaxed position of the atoms in z-direction. How much percent contraction we have for the two top most layers? This can be one of your results.

- As we discuss in the lecture the format of atomic positions in CONTCAR is in "Direct" format which you might not be comfortable with that. If so you can run the following program to convert your CONTCAR direct format to Cartesian.

  Command:

  ```
  Cartesian2Direct.x < [input file] > [output file]
  ```

  Example:

  ```
  Cartesian2Direct.x  <  CONTCAR  >  CONTCAR.car
  ```

  Note: do not forget to write the signs"<" and ">"

13. If you have time you can redo your calculation with a bigger unit cell along **a_3** and see if the total energy is different.

14. In order to see the forces on ions, transfer the file OUTCAR to your local computer, open the file by an editor and search for words "TOTAL-FORCE". How does the forces change at different ionic iterations? This can be also another result. You can for example plot one of the forces as a function of ionic iteration.

15. you can consult the results of the calculation with me.

• Adsorbate in the gas phase

1. Make the input file POSCAR in your local computer and calculate the adsorbate-adsorbate distance as close as possible to the value of 0.7Å 1.14Å for

H-H and CO respectively.

2. Make a separate folder for this calculation. Copy all necessary input file (the one which are for molecule calculation i.e. KPOINTS_for_H_molecule) from the either two folders: INPUT_FILES_for_H_adsorption_on_Pd or INPUT_FILES_for_CO_adsorption_on_Pd (depending on your project) to your new folder.
3. Rename them to proper input file name, i.e. rename INCAR_for_CO_molecule to INCAR file so that computer will use them as an INPUT file for VASP.
4. Transfer your POSCAR form your local computer to your new folder.
5. Do pdb to make a pdb format of your POSCAR, i.e. call it as POSCAR.pdb.
6. Transfer the pdb format file to your local computer. Using “raswin” obtain the distance between two molecules. Measure bond length distance to be sure they are the same as you have calculated.
7. Run VASP.
8. At the end of the program you will see the total energy of the slab and forces on each ion stored in OUTCAR. Look for the total energy in the last iteration. How much is it and what does this total energy mean? (you get another result)
9. The created file CONTCAR will give you the final position of the ions. Make a pdb format of this file (i.e. CONTCAR.pdb). Then transfer it to your local computer and view it by “raswin” and obtain the bond length. How much did it change? (You get another result)
10. In order to see the forces on ions, transfer the file OUTCAR to your local computer, open the file by an editor and search for words “TOTAL-FORCE”. How do the forces change at different ionic iterations?
11. If you are interested to find out the energies of each molecular orbitals it is written in the OUTCAR. Transfer the OUTCAR to your local computer and search for “band no” at the very end of the file. Each value below this line is the energy of every molecular orbital. Can you recognize the σ and π orbitals? (see reference number 4, page 28 if you are interested)

- **Calculation on Slab+adsorbate**

1. In this section you need to calculate the adsorption energy for at least two different high symmetry sites therefore you need to have two new folders, one for on-top site and one for hcp (for (111) surface) or hollow (for (100) surface) site. Consider on-top site first and make your POSCAR.

2. In order to locate your adsorbate on the substrate you need to have some initial position. It is good to have a good suggestion for adsorbate position. The following table shows the adsorbate-substrate bond-length (d1) for the high symmetry sites for (111) and (110) surfaces. Please try to take the adsorbate-metal distance as close as possible to the following distances. For simplicity the following table shows the distance between adsorbate and the Pd atom right below the adsorbate (d2).

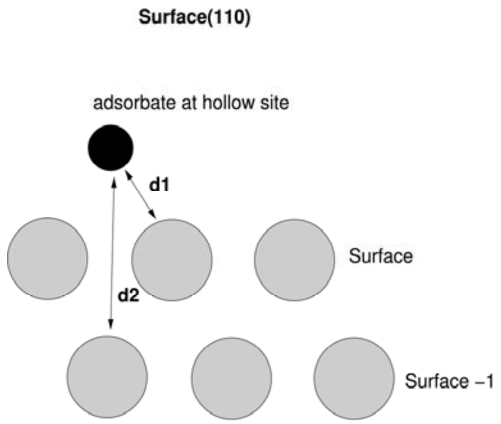
surface(111)

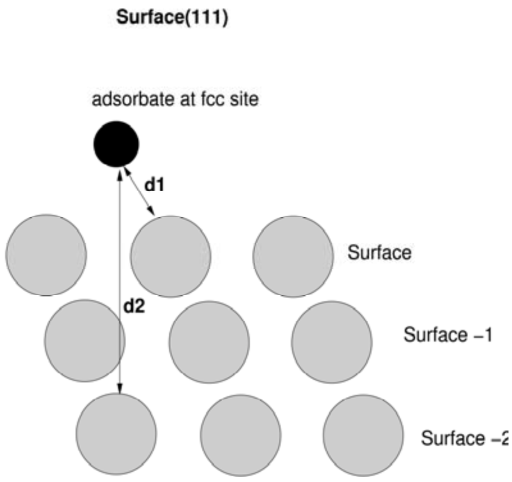
	Fcc 3-fold hollow site		On-top site
	d1	d2	
CO adsorbtion	2.07	5.93	1.87
Hydrogen adsorption	1.82	5.40	1.55

Surface(110)

	Fcc 3-fold hollow site		On-top site
	d1	d2	
CO adsorbtion	2.70(Pd-C)	2.43(Pd-C)	1.87(Pd-C)
Hydrogen adsorption	2.40	1.62	1.55

The distance between C and O in CO molecule in the gas phase is 1.14Å.
In the case of CO adsorption on the metal surface the carbon stays on the metal surface and oxygen stays on top of the carbon.





3. Follow the instruction from point 7 to 14 again.

4. Obtain the total energy of the system and calculate the adsorption energy as:

$$E_{ads}[CO] = E_{slab+CO} - E_{CO}$$

or

$$E_{ads}[H] = E_{slab+H} - \frac{1}{2}(E_{H2})$$

(derive the formula)

5. Make a pdb form of the CONTCAR and obtain the adsorbate-substrate bond-length and compare it with the table. If you are interested you can also check the distances between Pd atoms and compare it with the case of slab where there is no adsorbate. Are they different? (you get another result)

6. Transfer the OUTCAR to your local computer and obtain the forces on each ion at the last ionic iteration. They must be small enough.
7. Now you can consider hollow site in (100) surface (or fcc site for (111) surface) and follow the instruction from 1.

All results you have obtained in this instruction should be reported. Your report should contain an abstract, introduction, results, conclusions and reference.

Every group should have a project report. ☺

Good luck

Appendix

A. How to run the program vasp:

1. Login to pemfc
2. Prepare all the necessary input files into your work directory and if you have any output file from the previous run please delete them. Write “clnode” in the command line. This command will tell you which node is free for runing the vasp. Example:

```
aroudgar@pemfc:~/>  clnode
     fc02
```

This means that node number 2 is free.

3. run the commnad: cljob as following:

cljob [free node number] vasp

example:

```
aroudgar@pemfc:~/> cljob 2 vasp

R aroudgar  6563   0 18944 11:52 52.0 00:00:01 home/aroudgar/bin/vasp
```

The letter “R” at the beginning shows that the status of your program is “running”. The number at the left side is the id number of your job. This might be helpful when you want to kill your job.

4. In the case you want to kill your job run the following command: clsh [node number] kill –STOP [id number]

the node number must be the same as the node number you have entered at the beginning of the run.

B. How can we make sure that the program is running?

2. You can just write “ls” to see the list of the files including the output files. When you see the list of the output files then that means that the program has started to run.
3. Write “cljobs” in the commnad line. This will give you the id number of your job and the status of your job
4. Run the commnad tail with the option “-f” and then one of the output files, i.e. OSZICAR. Example:

```
tail -f OSZICAR
```

This command shows you the last lines of your OSZICAR and it waits for the new data from the computer until you cancel it by “ctrl”+“c”

Appendix C: Some simple Linux commands

For more information on each command in your SSH shell (putty) please type: man [name of the command]

```
   1. ls
                ls - list directory contents

         SYNOPSIS
                ls [OPTION]... [FILE]...

         DESCRIPTION
                List information about the FILEs (the current directory by
         default).
                Sort entries alphabetically if none of -cftuSUX nor --sort.

                OPTION

                -a,
                       do not hide entries starting with .


                -l     use a long listing format

   2. cd
               cd – Change the current directory to dir


         SYNOPSIS
                cd [dir]

         Note: “cd ..” can be used to go to the upper directory


3.    mkdir

                mkdir - make directories

         SYNOPSIS
                mkdir [OPTION] DIRECTORY...

         DESCRIPTION
                Create the DIRECTORY(ies), if they do not already exist.

                Mandatory arguments to long options are mandatory for short
         options too.

4.    rmdir

               rmdir – remove empty directories

         SYNOPSIS
```

```
        rmdir [OPTION] DIRECTORY...
```

5. cp

```
         cp - copy files and directories

   SYNOPSIS
          cp [OPTION]... SOURCE DEST
          cp [OPTION]... SOURCE... DIRECTORY
          cp [OPTION]... --target-directory=DIRECTORY SOURCE...

   DESCRIPTION
          Copy SOURCE to DEST, or multiple SOURCE(s) to DIRECTORY.

          Mandatory arguments to long options are mandatory for short
   options too.
```

6. pwd

```
        pwd – print name of current /working directory

   SYNOPSIS
        pwd [OPRTION]
```