

E. Surface Reconstruction of Si(001)

Despite the enormous progress in experimental surface science, notably with spectroscopic methods exploiting synchrotron radiation and scanning tunneling microscopy, computations remain one of the most useful sources for accurate data on surface structures. In fact, quite often it is the combination of experimental and computed results, which gives the most reliable data of surface structures. As an example, let us apply MEDEA to the Si(001) surface. This surface is the typical substrate in the manufacturing of semiconducting devices.

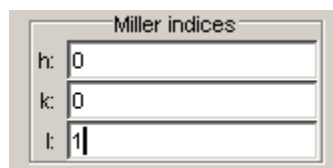
1. Retrieve Bulk Si Structure

Using INFOMATICA, search for “**Formula is Si**”, select **ICSD.76268** and **View structure**.

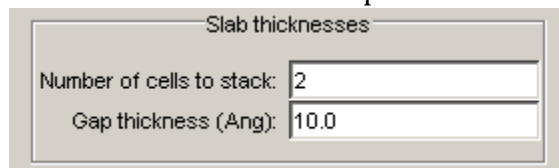
2. Optimize Lattice Parameters of Bulk Si

Using the Si structure retrieved from INFOMATICA select **VASP 4.6** >> **Run** and perform a **Structure Optimization** (check **Relax atom positions**, **Allow cell shape to change**, and **Allow cell size to change**) with **Accurate** precision. Leave the remaining parameters at their default and launch the calculation. The lattice parameter increases from the initial value of 5.43086 Å by 0.7% to 5.469643 Å.

3. Create Surface

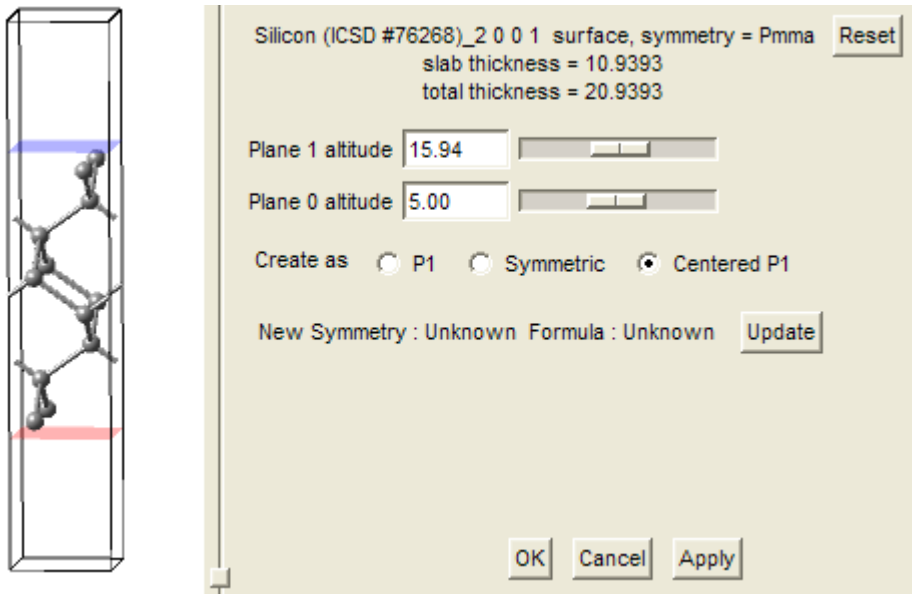


Miller indices	
h:	0
k:	0
l:	1

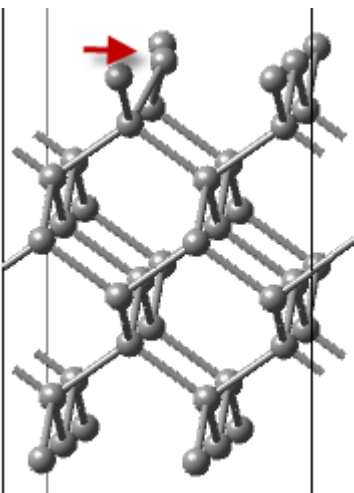


Slab thicknesses	
Number of cells to stack:	2
Gap thickness (Ang):	10.0

Use **File** >> **Open** >> **Previous Calculation** to load the optimized structure of bulk Si. From the MEDEA menu bar, select **Edit** >> **Build surfaces ...** and define Miller indices 0 0 1 and click on **Search**. The system creates a new unit cell with the (001) plane parallel to the xy-plane. You can select the number of cells to stack in the z-direction as well as the gap between the slabs. In the present case, leave the values at their defaults as shown on the left side. Use **Create** to open a new window with two panels.



Rotate the newly created structure in the upper panel to see the supercell, which is a surface model of the Si(001) surface. The sliders in the lower panel allow the trimming of the surface.



Click on **Update** to determine the symmetry of the system. In the present case, this is Pmma. Leave the defaults and select **Create Centered P1** and confirm with **OK**.

This action generates a new structure in a new window. Select this new structure and create a 2x2x1 supercell by using **Edit** >> **Build supercells...**

The resulting structure is shown on the left.

Select the surface atom marked by an arrow and move it from $x=0.375$ to $x=0.45$. This breaks the symmetry of the surface and we can now launch an optimization.

4. Set-up and launch VASP Calculation

Make sure that the structural model with the displaced surface atom is selected in the MEDEA window. Choose **VASP 4.6** >> **Run** from the MEDEA tool bar. Choose **Structure Optimization** as the type of calculation. Only the box **Relax atom positions** should be checked. Choose **Normal** accuracy. Leave all other parameters at their default and hit the **Run** button.

Analyze Results

Once the calculation is finished (on an AMD Opteron processor, this takes about 2 hours), retrieve the optimized structure from **File** >> **Open** >> **Previous Calculation**. As shown below, the surface Si atoms form surface dimers with the bond axis tilted with respect to the (001)

plane. Within a row, the tilt angles alternates. Note that also the lower surface of the slab model shows this reconstruction, although only one atom at the top surface has been moved initially.

