Zacros Tutorial 2: Creating Lattice Input for Pt(100)

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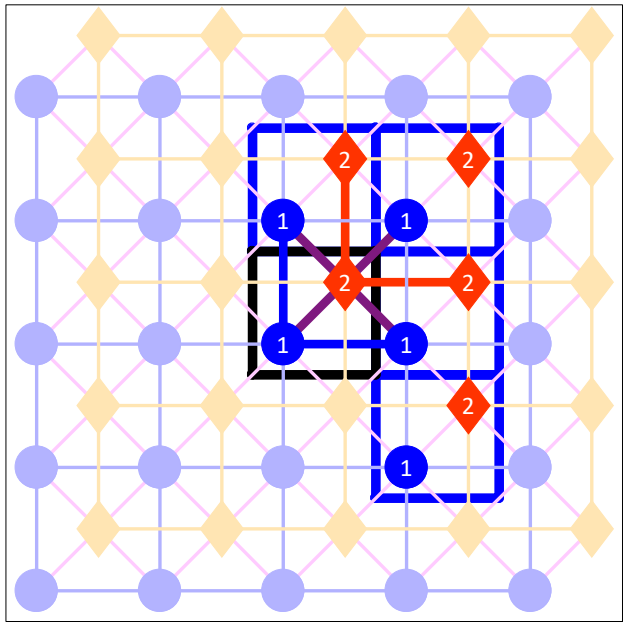
FCC(100) Lattice Input File

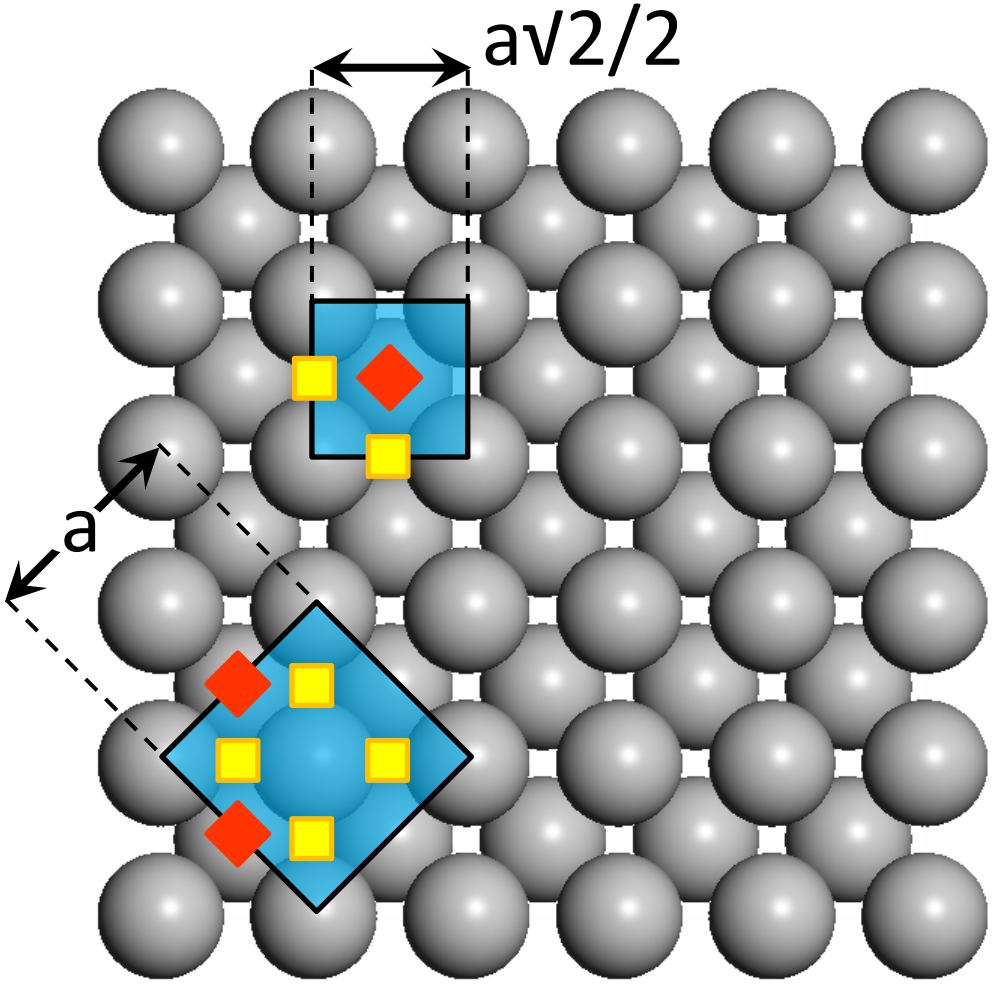
```
lattice periodic_cell
cell_vectors # in row format (Angstroms)
    2.751140353562500 0.000000000000000
    0.000000000000000 2.751140353562500
repeat_cell      7 7
n_site_types     2
site_type_names  top hol
n_cell_sites     2
site_types       top hol
site_coordinates # fractional coord. (x,y) in rows
    0.250000000000000 0.250000000000000
    0.750000000000000 0.750000000000000

neighboring_structure # site-neighsite cell
    1-2 self
    1-1 north
    1-1 east
    2-1 north
    2-1 northeast
    2-1 east
    2-2 north
    2-2 east
end_neighboring_structure

end_lattice
```



- In the 1st tutorial, we prepared an input file for Pd(100) with atop and 4-fold hollow sites.

A Slightly Different Lattice Structure

- Let us now suppose that we want a lattice with bridge and 4-fold hollow sites only…



… because in the system we want to simulate, these are the sites on which our adsorbates bind most strongly.

a = 3.924 Å for Pt

hollow

bridge

Activity

- Choose one out of the two unit cells drawn in the previous slide and set up the **`lattice_input.dat`** file. For guidance, you can use: the slides of the first tutorial of this workshop, the manual, and the online tutorial: http://zacros.org/tutorials/11-lattice-input-for-a-fcc-100-surface
- Create a very simple **`simulation_input.dat`** file (you can use the one of tutorial 1), place it in the same directory as the lattice input file, and run *Zacros*. Check that these files are parsed without errors (you are expected to get an error that other input files are missing).
- Plot the lattice output with the Matlab script provided.