Computational Materials Physics

Center for
Molecular
Modeling

Department of
Materials Science
and Engineering

supercells
(impurities and surfaces)

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http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

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the supercell concept

Put a single atom in an otherwise empty, big unit cell:

10-15 Å

fcc Bravais lattice:
12 "nearest" neighbours =
as spherically symmetric as possible.
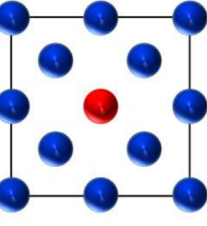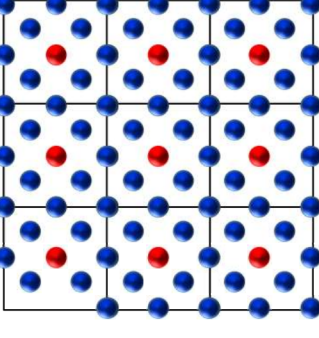
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the supercell concept

Replicate the chemical unit cell (here 2x2 in 2D) and replace one atom by an impurity:

the supercell concept

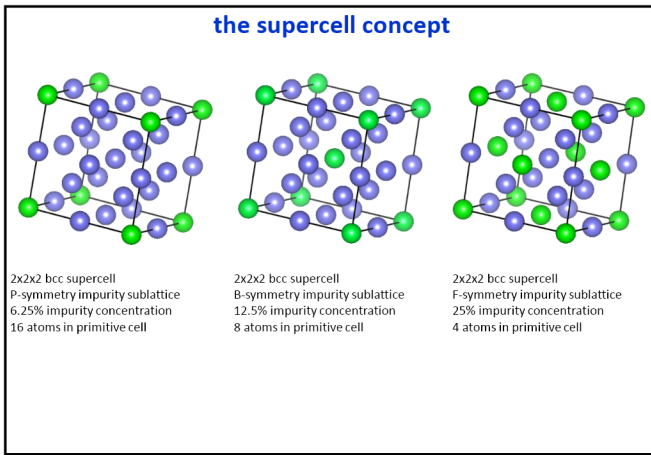2x2x2 bcc supercell
P-symmetry impurity sublattice
6.25% impurity concentration
16 atoms in primitive cell

2x2x2 bcc supercell
B-symmetry impurity sublattice
12.5% impurity concentration
8 atoms in primitive cell

2x2x2 bcc supercell
F-symmetry impurity sublattice
25% impurity concentration
4 atoms in primitive cell

surfaces

Inserting vacuum in a supercell results in slabs ➔ surfaces

example: Fe(001)

1x1x1 = 3 layers   1x1x2 = 5 layers   1x1x3 = 7 layers

expanded view
(7 layers)

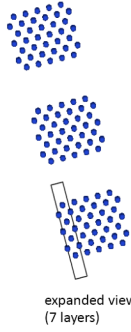## example: Fe(001)

new convergence criteria to be checked
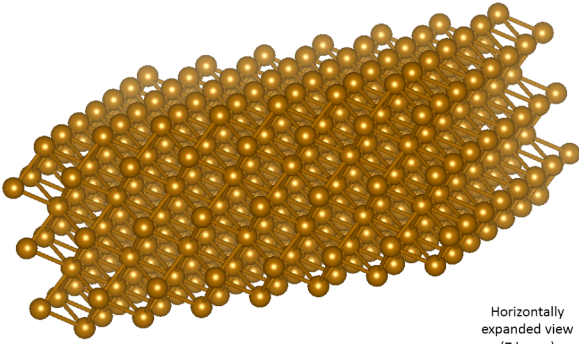for a physically relevant model :

- slab thickness
- vacuum thickness

expanded view
(7 layers)

example: Fe(001)

Horizontally
expanded view
(7 layers)
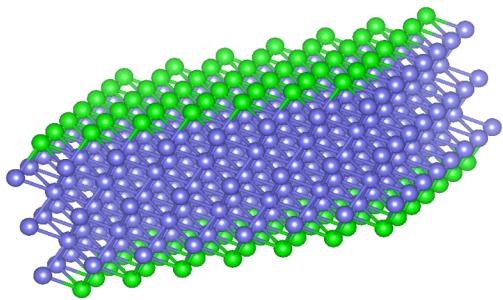
how to model a surface covered by a monolayer of
another phase? (=extremely thin coating)
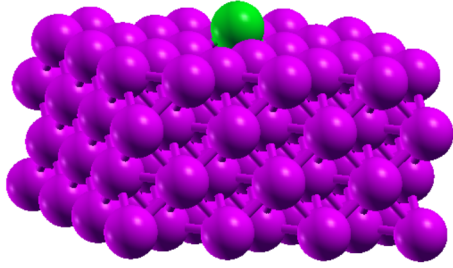
how to model a surface with an isolated impurity atom attached to it? (=adsorbate)