tutorial session XI

Properties

Atoms are characterized by:

Type, x, y, z, ADP, Property_flag

The Property flag is a binary sum of

N = **normal** instead of a void

M = Part of a **molecule** or not

D = Part of a **domain** or not

O = **outside** crystal surfaces or inside

E = Close to an **external** surface or not

I = Close to an **internal** surface or not

L = Atom is part of a **ligand** molecule

Property flags are set/changed when:

Reading; Inserting a domain; creating an external surface; removing an atom

Global Property selection rules are set with:

```
property
    property  ignore,  all
    property  present, normal
    property  absent,  domain
    property  ignore,  internal
exit
```

N = **normal** instead of a void

M = Part of a **molecule** or not

D = Part of a **domain** or not

O = **outside** crystal surfaces or inside

E = Close to an **external** surface or not

I = Close to an **internal** surface or not

L = Atom is part of a **ligand** molecule

Global property selection rules apply:

- replace
- mmc
- find_env

(More under construction...)

Local property selection rules apply:

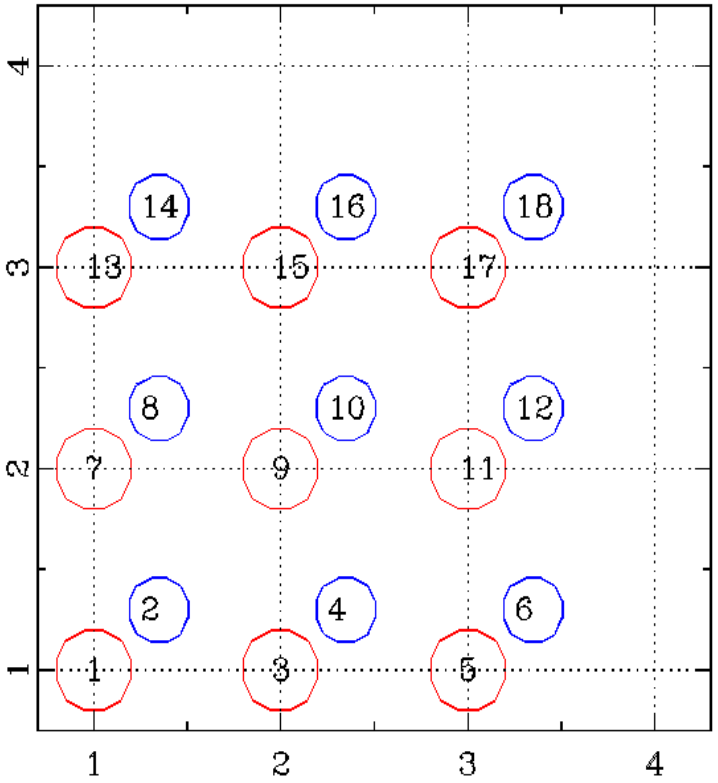
- plot menu
- save

(More under construction...)

User defined Property selection rules are set with:

```
property
!    Silicon that has 2 to 6 neighbors in its connectivity 1
     property  present, atom:Si, conn:1, nmin:2, nmax:6
!
!    Silicon that does not have 2 to 6 neighbors
!    in its connectivity 2
     property  present, atom:Si, conn:2, emin:3, emax:4
!
!    ignore = clear user definition number 1
     property  ignore,  no:1
!
!    ignore = clear all global and user definitions
     property  ignore,  all
exit
```

Y - axis



X - axis

Seqence of atoms in perfect:

Within each unit cell == sites

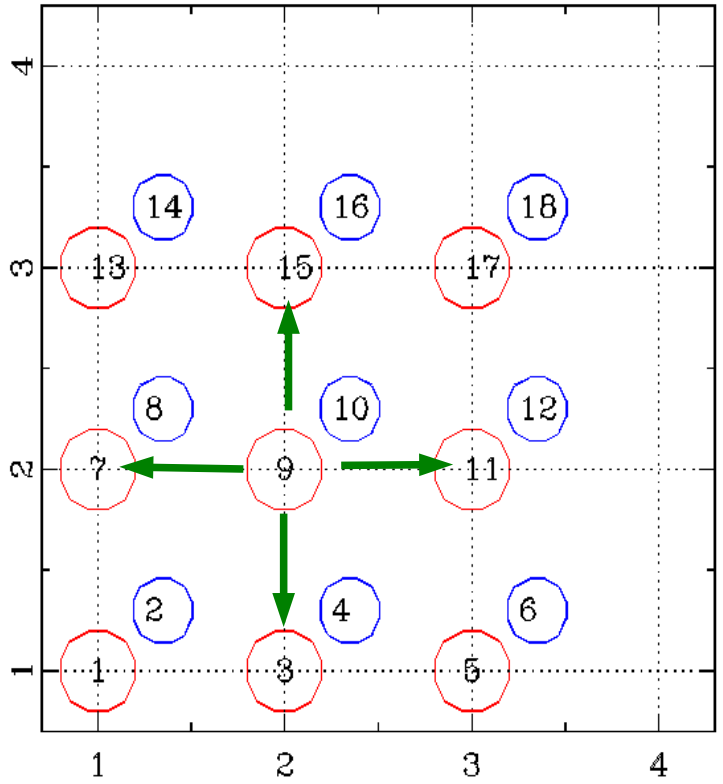
Unit cells along x

Unit cells along y

Unit cells along z

All **red** atoms on site 1
All **blue** atoms on site 2

Y - axis



X - axis

Neighbors for atom 9

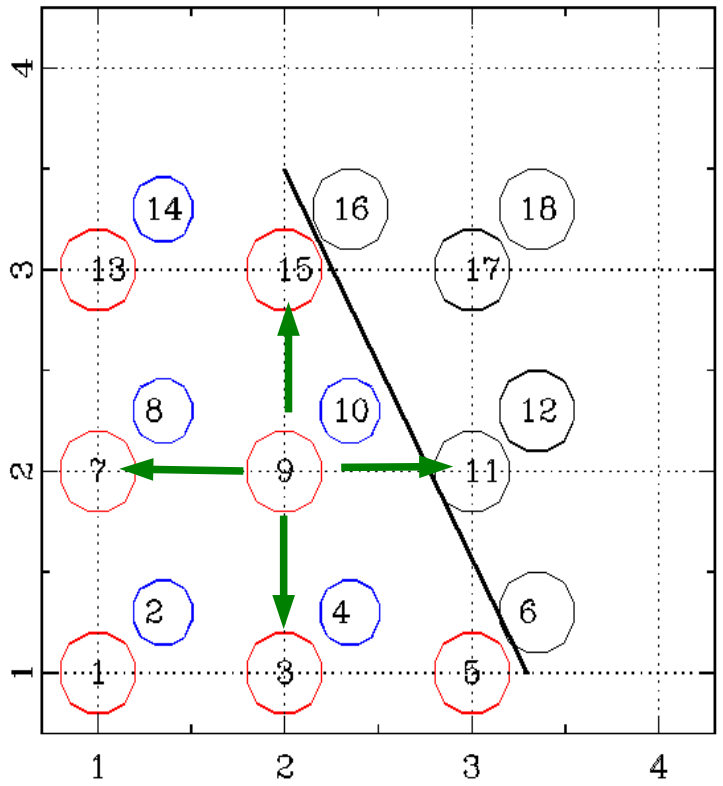
3: site 1 in [0, -1, 0]
7: site 1 in [-1, 0, 0]
11: site 1 in [1, 0, 0]
15: site 1 in [0, 1, 0]

in „chem“ and „mmc“ menus

set vect, 1, 1, 1, 0,-1, 0
set vect, 2, 1, 1, -1, 0, 0
set vect, 3, 1, 1, 1, 0, 0
set vect, 4, 1, 1, 0, 1, 0

This will describe ALL neighbors
of site 1 in any unit cell!
Very fast algorithm to address atoms!

Y - axis



X - axis

Nothing has changed, voids are „regular“ atoms

Some atoms removed, still in memory!

Neighbors for atom 9

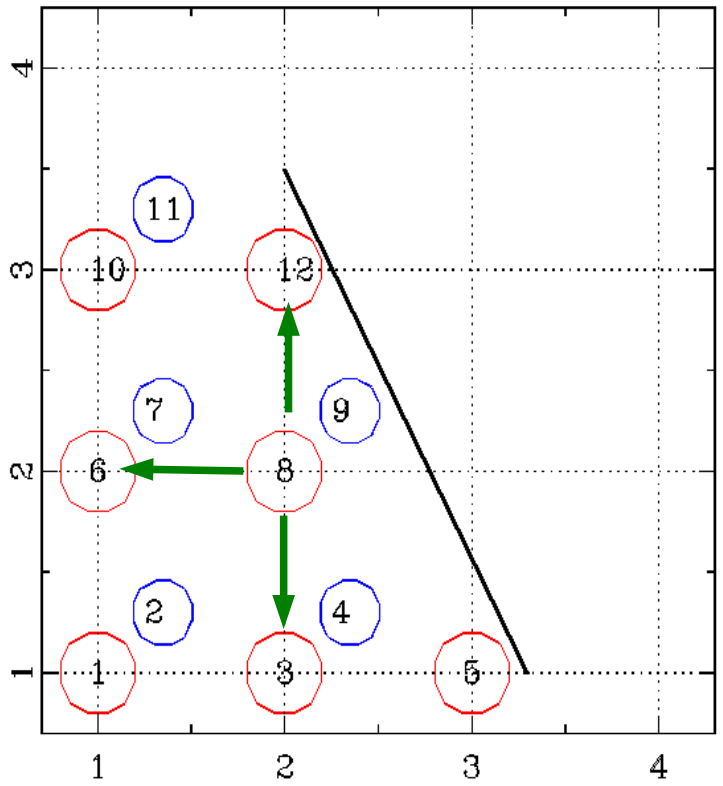
3: site 1 in [0, -1, 0]
7: site 1 in [-1, 0, 0]
11: site 1 in [1, 0, 0]
15: site 1 in [0, 1, 0]

in „chem“ and „mmc“ menus

set vect, 1, 1, 1, 0,-1, 0
set vect, 2, 1, 1, -1, 0, 0
set vect, 3, 1, 1, 1, 0, 0
set vect, 4, 1, 1, 0, 1, 0

This will describe ALL neighbors
of site 1 in any unit cell!
Very fast algorithm to address atoms!

Y - axis



X - axis

Some atoms removed; **purge**

Neighbors for atom 9 → 8!

3: site 1 in [0, -1, 0]	3!
7: site 1 in [-1, 0, 0]	6!
11: site 1 in [1, 0, 0]	
15: site 1 in [0, 1, 0]	12!

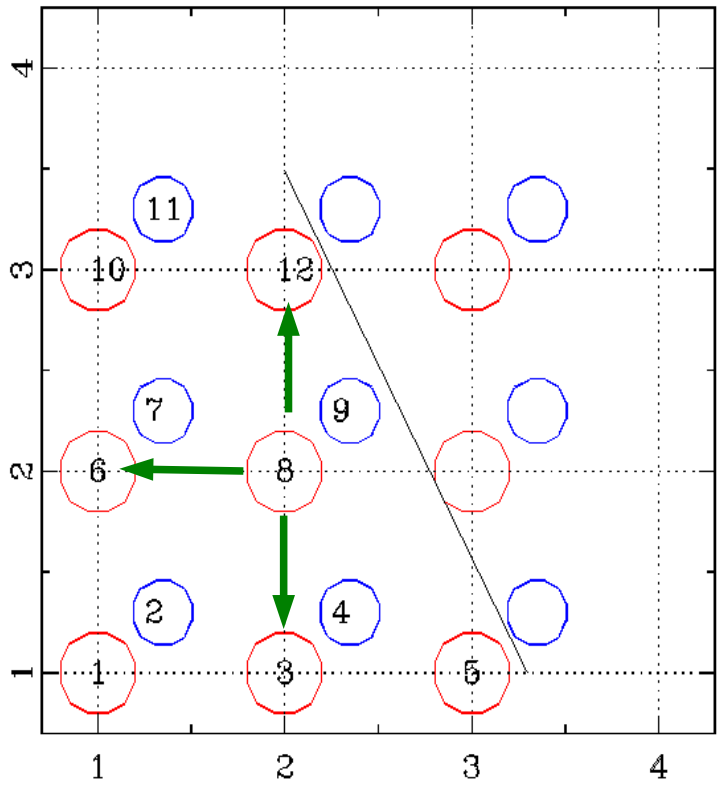
in „chem“ and „mmc“ menus

set vect, 1, 1, 1, 0,-1, 0
set vect, 2, 1, 1, -1, 0, 0
set vect, 3, 1, 1, 1, 0, 0
set vect, 4, 1, 1, 0, 1, 0

This will describe ALL neighbors
of site 1 in any unit cell!
Very fast algorithm to address atoms!

Sequence of unit cells has changed !!!

Y - axis



X - axis

Explicit list of neighbors for EACH atom

Atom 1: 3; 6
Atom 3: 1; 5; 8
Atom 5: 3
Atom 6: 1; 8; 10
Atom 8: 3; 6; 12
Atom 10: 6; 12
Atom 12: 8; 10

Selection rules are:

Atom type
Distance range (rmin; rmax)

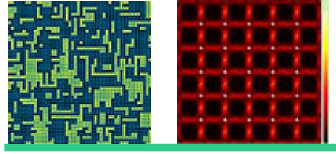
This will describe ALL neighbors
For each individual atom
Very fast algorithm to address atoms!

```
connectivity
    reset
    add cu,    cu, al, 0.2, 2.5, cu_first
    add O,     cu, al, 0.2, 2.5, ox_first
!   add central, neig1, …, rmin, rmax, descriptive_name
    show
    create
exit
```

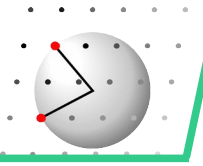
May take a while to create
Very fast application in mmc
Neighbors remain grouped even if actual distance changes

Start discus_suite
Select directory Lectures\06_Properties

suite> **@prop_ex_1.mac**



Exercise 1



Start discus_suite
Select directory Lectures\06_Properties

suite> **@prop_ex_2.mac**