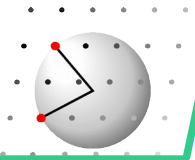




tutorial session XI

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

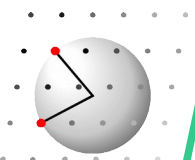
E = Close to an **external** surface or not

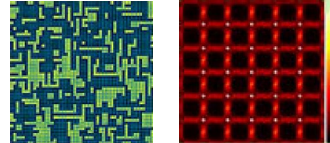
I = Close to an **internal** surface or not

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





Properties



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:

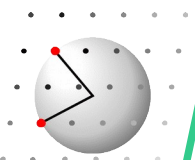
```
replace
mmc
find_env
```

(More under construction...)

Local property selection rules apply:

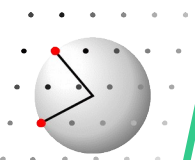
```
plot menu
save
```

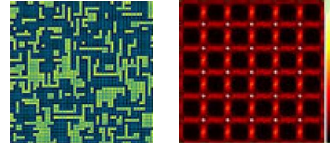
(More under construction...)



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
```

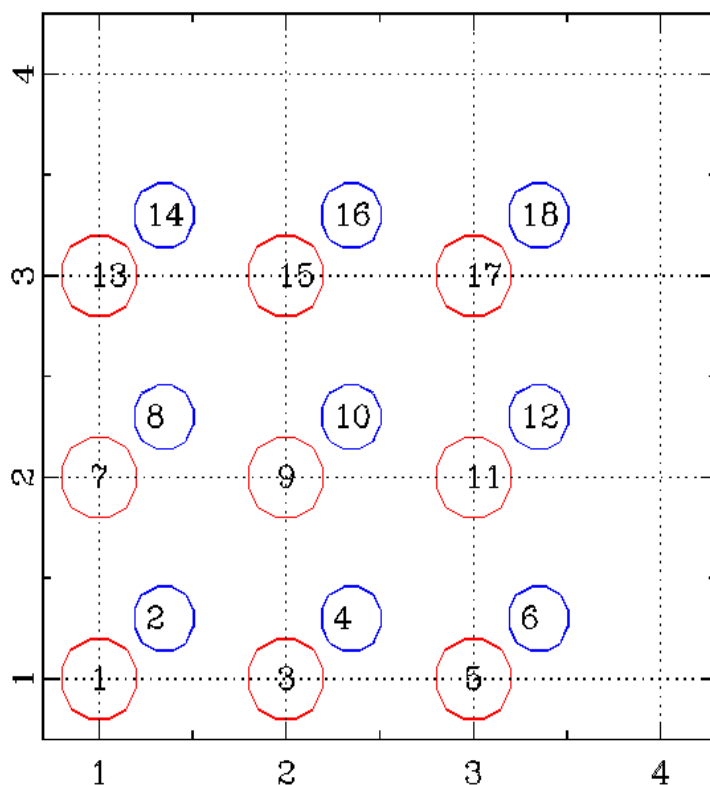




DISCUS numbering scheme



Y - axis



X - axis

Sequence of atoms in perfect:

Within each unit cell == sites

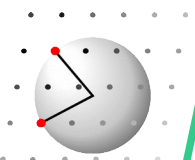
Unit cells along x

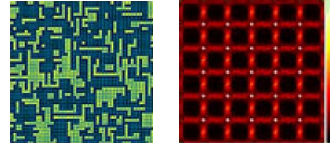
Unit cells along y

Unit cells along z

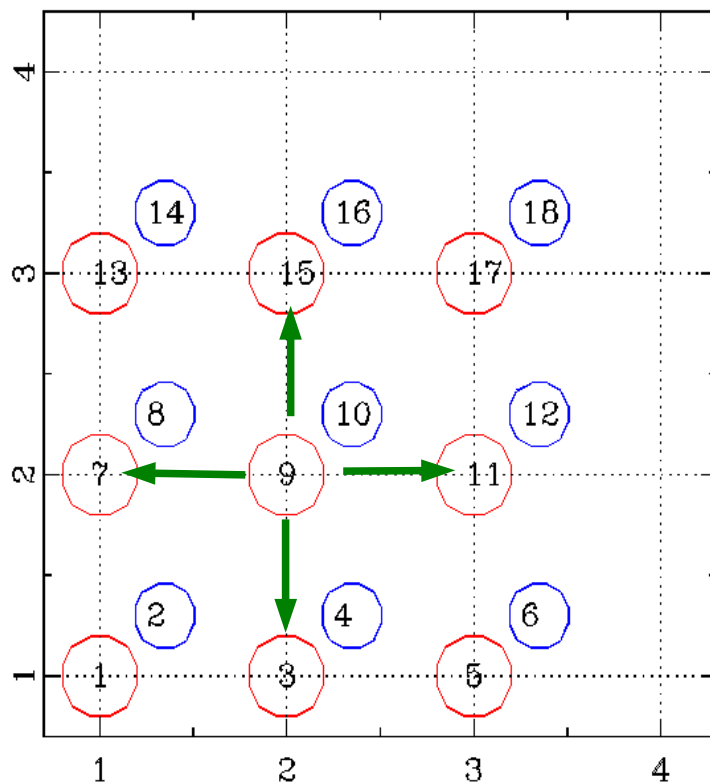
All **red** atoms on site 1

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

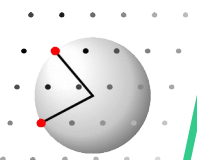
set vect, 2, **1**, **1**, -1, 0, 0

set vect, 3, **1**, **1**, **1**, 0, 0

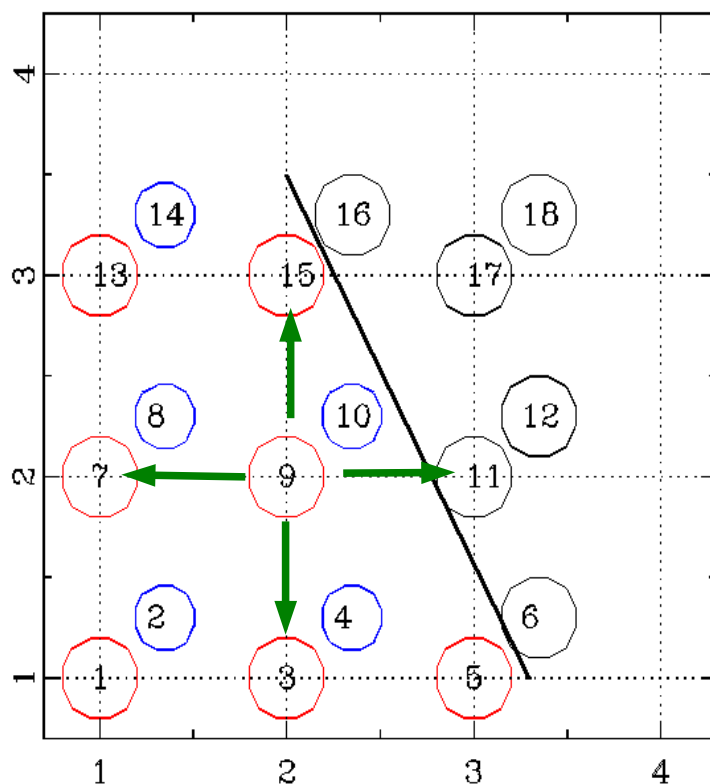
set vect, 4, **1**, **1**, **0**, 1, 0

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**

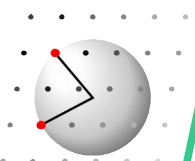
set vect, 2, **1**, **1**, **-1**, **0**, **0**

set vect, 3, **1**, **1**, **1**, **0**, **0**

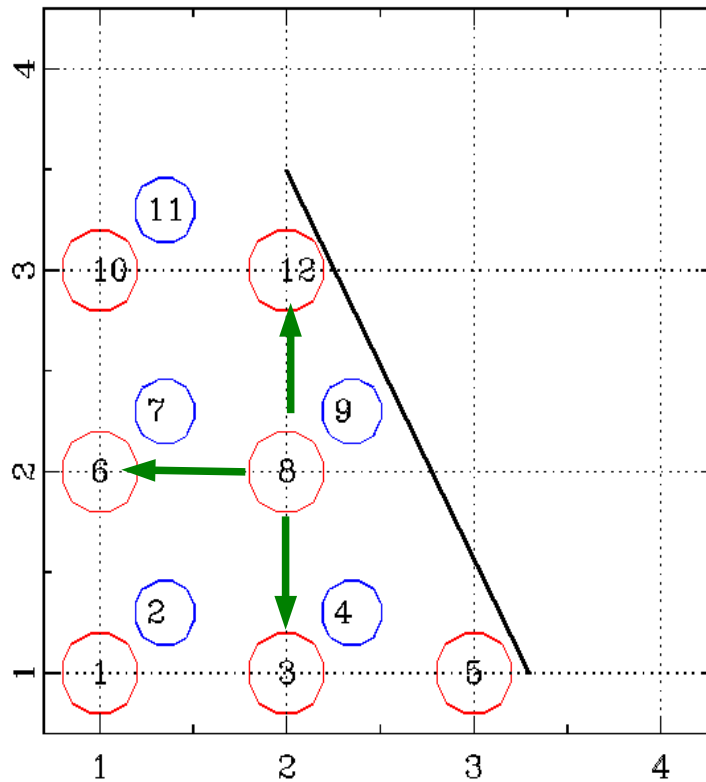
set vect, 4, **1**, **1**, **0**, **1**, **0**

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!

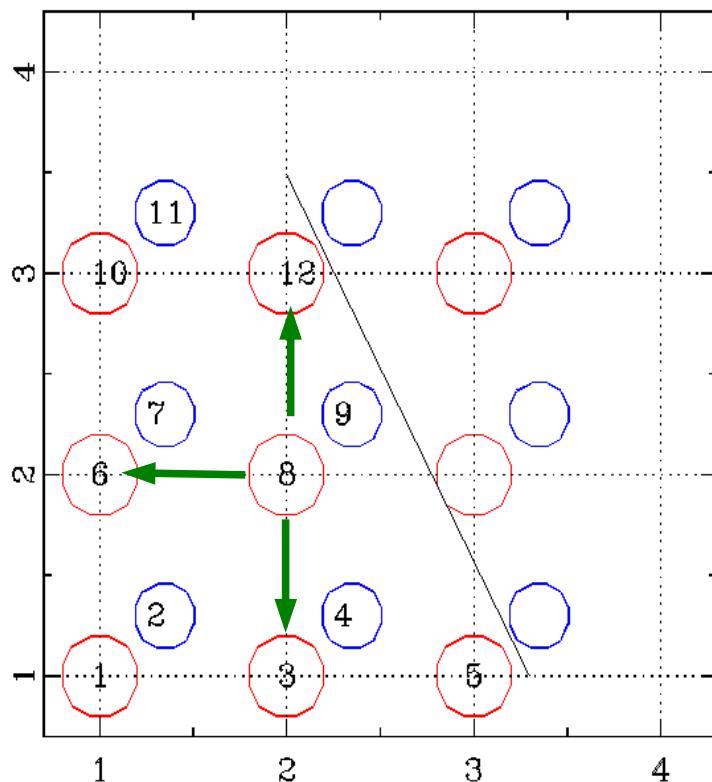
Sequence of unit cells has changed !!!



DISCUS connectivity scheme



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:

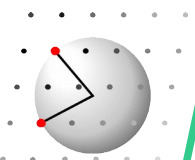
Atom type

Distance range (rmin; rmax)

This will describe ALL neighbors

For each individual atom

Very fast algorithm to address atoms!





Exercise 1

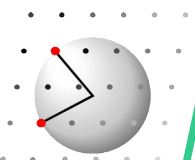


```
connectivity
  reset
  add cu,    cu, al, 0.2, 2.5, cu_first
  add O,     cu, al, 0.2, 2.5, ox_first
!  add central, neig1, ..., rmin, rmax, descriptive_name
  show
  create
exit
```

May take a while to create

Very fast application in mmc

Neighbors remain grouped even if actual distance changes



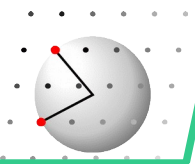


Exercise 1



Start discus_suite
Select directory Lectures\11.Properties

suite> [@prop_ex_1.mac](#)



Exercise 1



Exercise 2



Start discus_suite
Select directory Lectures\11.Properties

suite> [@prop_ex_2.mac](#)

