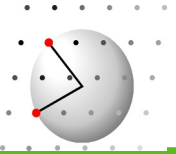# DISCUS Workshop
Strain

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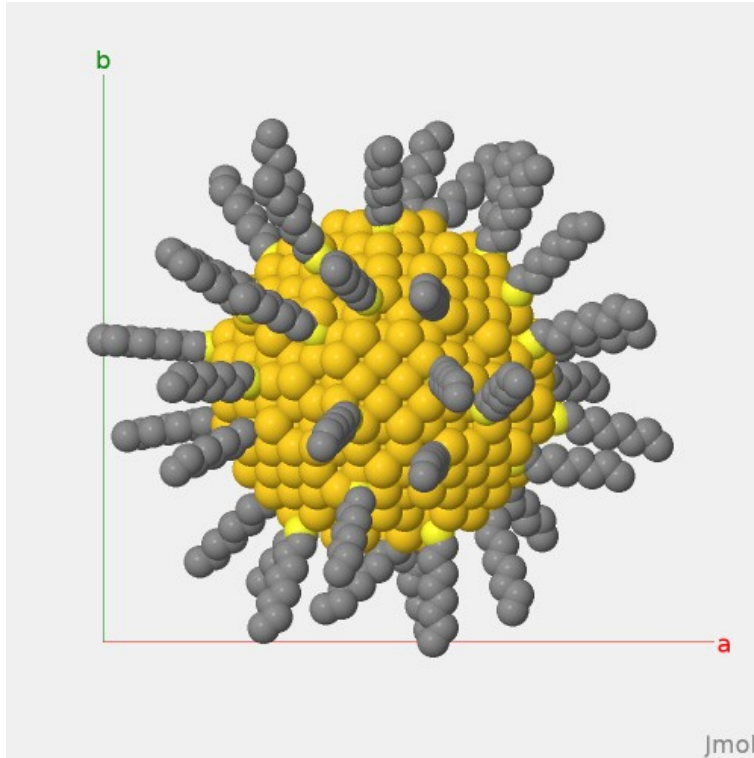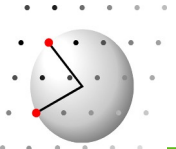
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Building a **strained** Nanoparticle

Goal:
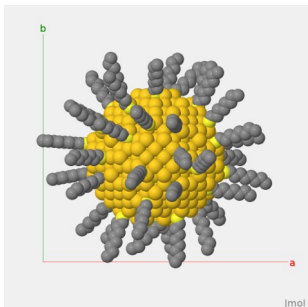
Build an ellipsoidal Gold nanoparticle decorated with a simple ligand

Introduce strain by Au-S-Au bond angle

Basic Concept:

Define relationship to neighboring atoms

Use a force field to relax structure

Related menus
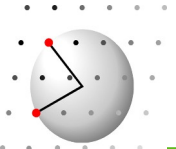
mmc :   **General Multiple-Monte-Carlo**
                 Defines neighbors
                 Defines modification scheme
                 Relaxes structures

connectivity: **Defines neighbors in distance shells**

neigbourhood   which atoms are correlated
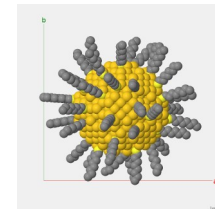   distance, list of interatomic vectors, ...

correlations   how are atoms related to each other ?
                              different energy terms
                              chemical   equal atoms <==> different
                              distance   distance between atom pairs
                              angular   bond angle in triplet

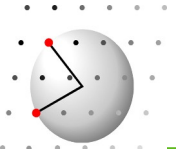modification   how is the crystal structure changed
                              switch two atoms
                              shift individual atoms

Monte Carlo   details of the process
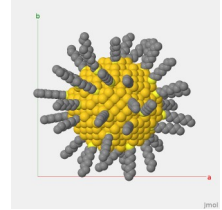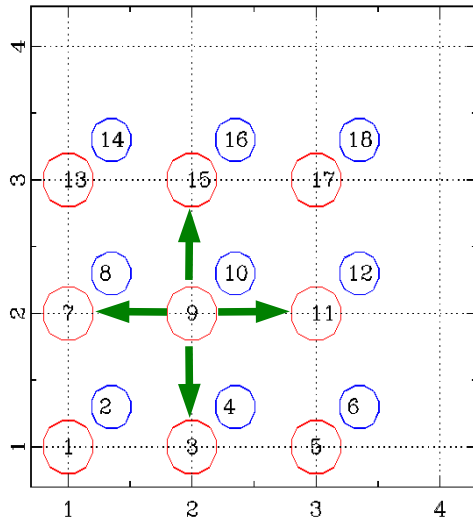   number of refinement cycles
                              pseudotemperature kT

neigbourhood

which atoms are correlated
distance, list of interatomic vectors, ...

Red 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]**

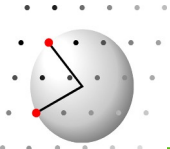15: site 1 in **[0, 1, 0]**

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**
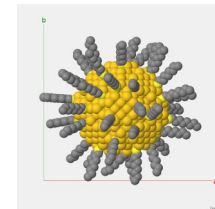
Y - axis

X - axis

Internal sequence

neigbourhood

which atoms are correlated
distance, list of interatomic vectors, ...
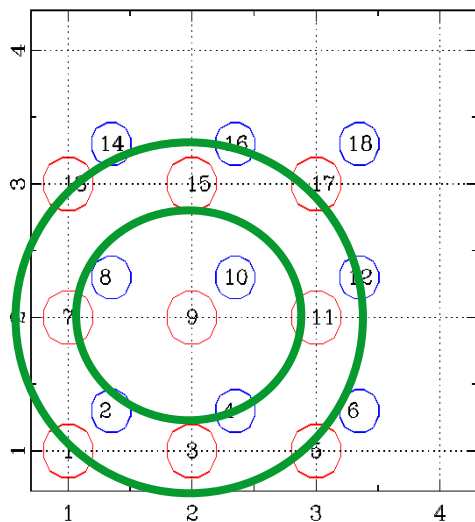
Neighbors for atom 9

3; 7; 11; 15:
Atoms of type **red** in
distance shell

Y - axis

Connectivity menu

X - axis

Internal sequence
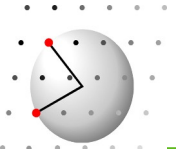
Commands:

add central, neighbor(s), distances, name   Define type and distance range
create   Create all the lists

Options for **add**

"**first**:<**number**>"   Restrict list to the shortest <number> distances
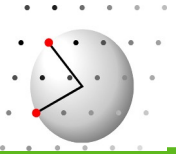"**molescope**:**within**"   Restrict to distances in the same molecule
"**molescope**:**outside**"   Restrict to distances to other molecules
"**molescope**:**ignore**"   Use any distance pair

neigbourhood   which atoms are correlated
                        distance, list of interatomic vectors, ...

strain.mac


```
connectivity
  reset
  add Au, Au, 2.5, 2.9, au_au_first ! Build Gold-Gold neighbor list
  add S,  Au, 2.0, 2.5, s_au_first  ! Build Gold-Sulfur list
  create                            ! Perform the actual creation
exit
```
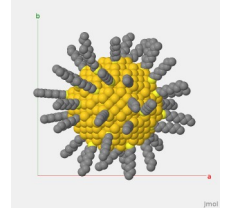
neigbourhood   which atoms are correlated
                         distance, list of interatomic vectors, ...
                    strain.mac

```
connectivity
  add Au, Au, 2.5, 2.9, au_au_first ! Build Gold-Gold neighbor list
  add S,  Au, 2.0, 2.5, s_au_first  ! Build Gold-Sulfur list
  create                            ! Perform the actual creation
exit
#
mmc                                 ! Multiple Monte-Carlo menu
  reset                             ! Back to start up conditions
  set con, res                      ! Remove previous connectivities
  set nei, res                      ! Remove previous eighborhoods
#
  set con, 1, Au,  au_au_first ! Use connectivity au_au_first
  set con, 2, S,   s_au_first  ! Use connectivity au_au_first
#
```
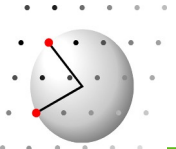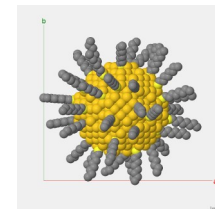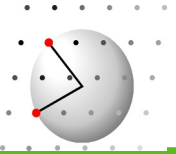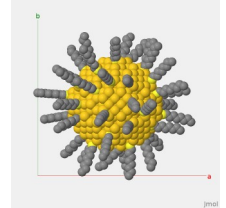
neigbourhood

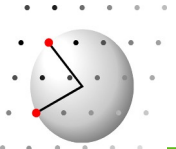which atoms are correlated
distance, list of interatomic vectors, ...

strain.mac

```
mmc                                  ! Multiple Monte-Carlo menu
  reset                              ! Back to start up conditions
  set con, res                       ! Remove previous connectivities
  set nei, res                       ! Remove previous eighborhoods
#
  set con, 1, Au,  au_au_first ! Use connectivity au_au_first
  set con, 2, S,   s_au_first  ! Use connectivity au_au_first
#
  set neig, number:next, con, 1    ! Au-Au distances
  set neig, number:next, con, 2    ! S-Au distances
  set neig, number:next, con, 2    ! Au-S-Au angles
#
```

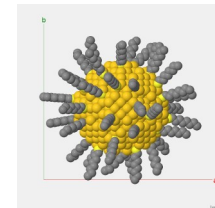A **neigbourhood** consists of one or several relationships (vectors, connectivities…)
All atoms in a (combined) neighborhood will contribute to an *energy* term
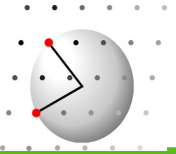
correlations   how are atoms related to each other ?
                      different energy terms

```
mmc          strain.mac          ! Multiple Monte-Carlo menu
  set con, 1, Au,  au_au_first ! Use connectivity au_au_first
  set con, 2, S,   s_au_first  ! Use connectivity au_au_first
#
  set neig, number:next, con, 1    ! Au-Au distances  no. 1
  set neig, number:next, con, 2    ! S-Au distances   no. 1
  set neig, number:next, con, 2    ! Au-S-Au angles   no. 1
#
  set target, 1, lennard, Au, Au, P_auau, D_auau, 12, 6 ! Au-Au distance
  set target, 2, lennard, S , Au, P_s_au, D_s_au, 12, 6 ! S-Au distance
  set target, 3, angle, S , Au, Au, P_angle, D_angle    ! Au-S-Au angle
#
```
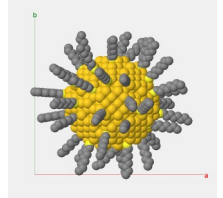
A **target** describes the *energy* to be minimised for all atom pairs in a neighborhood

Monte Carlo   Details of the process...

```
mmc                    strain.mac              ! Multiple Monte-Carlo menu
  set cyc, 500*n[1]                            ! On average, shift each atom 5000 times
  set feed,auto                                ! Feedback interval or 50*n[1]
  set temp,heat                                ! High temp will accept many "bad" moves
  set finish, stop:converge, diff:0.095, change:0.052, &
              aver:0.050, feed:3

#
```
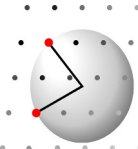
cycle: modify a single atom
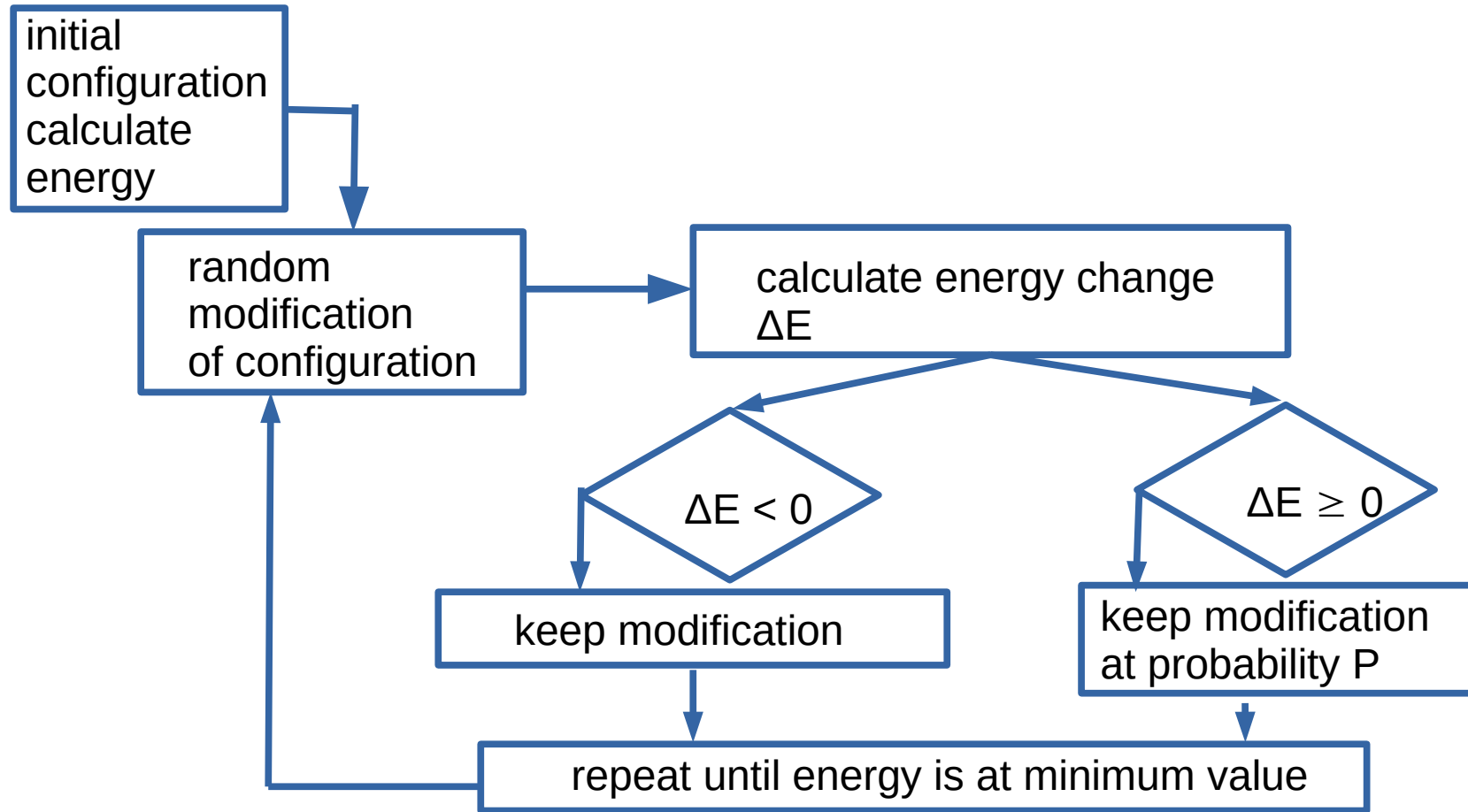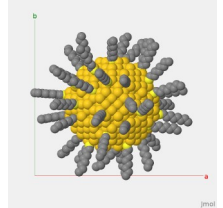
feedback: display current status; update internal parameters
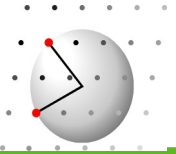
temperature: controls acceptance of wrong moves

finish: controls convergence

initial configuration calculate energy

random modification of configuration

calculate energy change ΔE

ΔE < 0

ΔE ≥ 0

keep modification

keep modification at probability P

repeat until energy is at minimum value

Metropolis et al. J. Chem. Phys. **21**, 1087-1092 (1953)

Monte Carlo   Details of the process...

```
mmc                    strain.mac              ! Multiple Monte-Carlo menu
  set cyc, 500*n[1]                            ! On average, shift each atom 5000 times
  set feed,auto                                ! Feedback interval or 50*n[1]
  set temp,heat                                ! High temp will accept many "bad" moves
  set finish, stop:converge, diff:0.095, change:0.052, &
               aver:0.050, feed:3
```

#

cycle: modify a single atom

feedback: display current status; update internal parameters

temperature: controls acceptance of wrong moves

finish: controls convergence