Institut Català
de Nanociència
i Nanotecnologia

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Molecular dynamics using SIESTA*

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*Based on previous presentations from Emilio Artacho and Marivi Fernandez-Serra, which can be found in the SIESTA webpage

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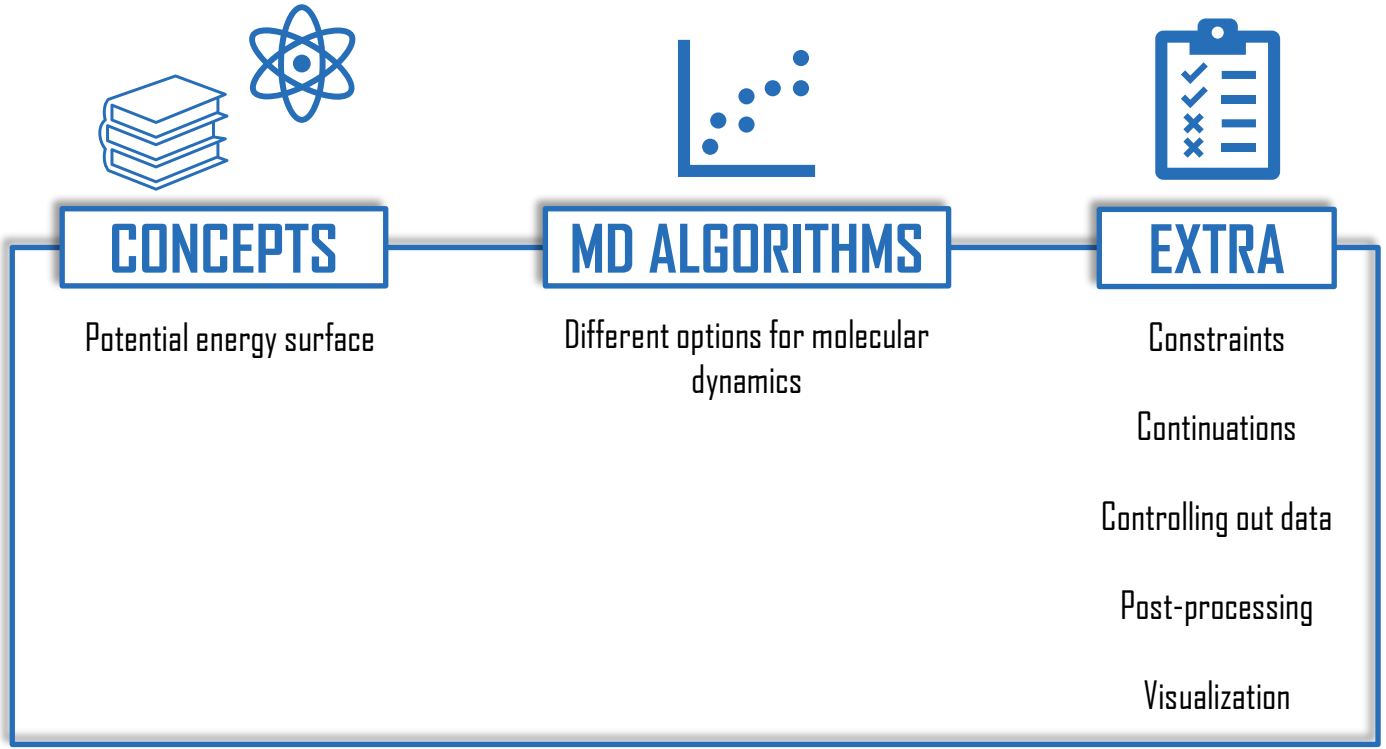
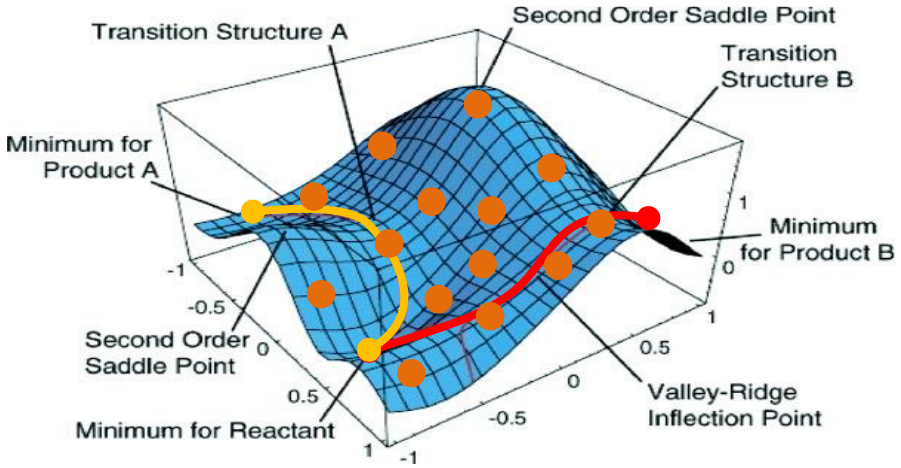
What is this presentation about?

Outline



The potential energy surface - PES

Geometry optimization x molecular dynamics



$$\text{Reactants} \xrightarrow{TS_A} A$$

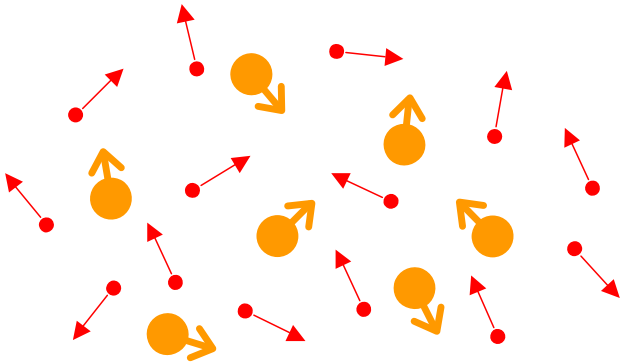
$$\text{Reactants} \xrightarrow{TS_B} B$$

Geometry optimizations	Molecular dynamics
We move on the PES	We move over the PES
Search for local/global minima	Sampling

Schlegel, H. B. J. Comput. Chem. (2003)

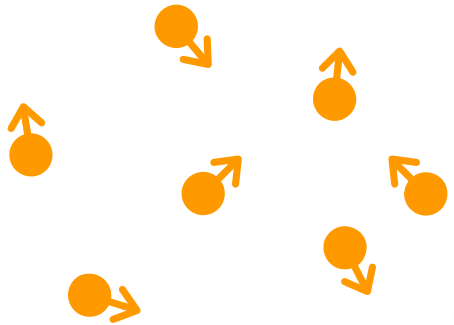
Adiabatic decoupling

Many body problem and how to move atoms



$$\frac{m_n}{m_e} \gg 1$$

Moving atoms



Need for computing the $\vec{F}$

Hellman-Feynman theorem

Algorithms for molecular dynamics

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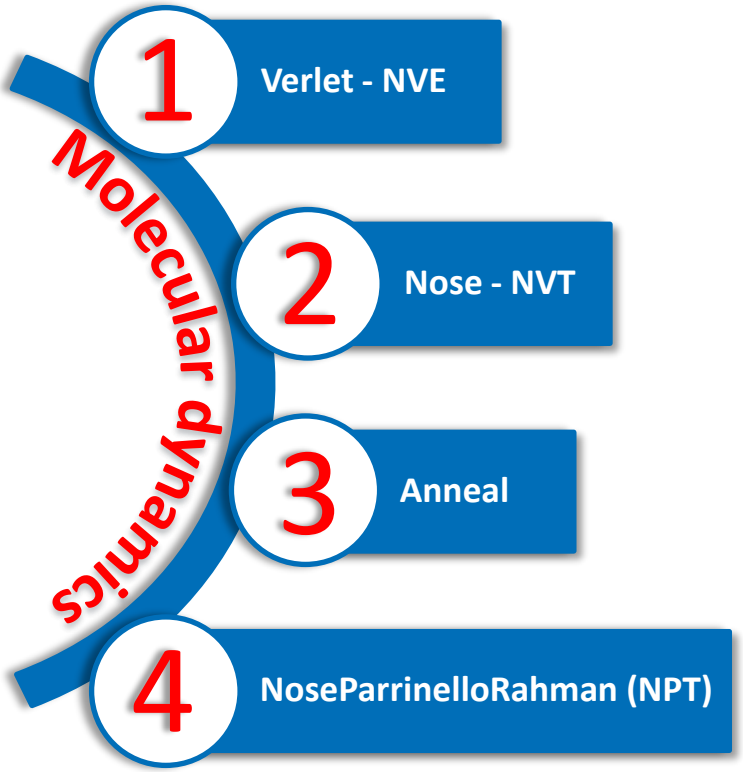
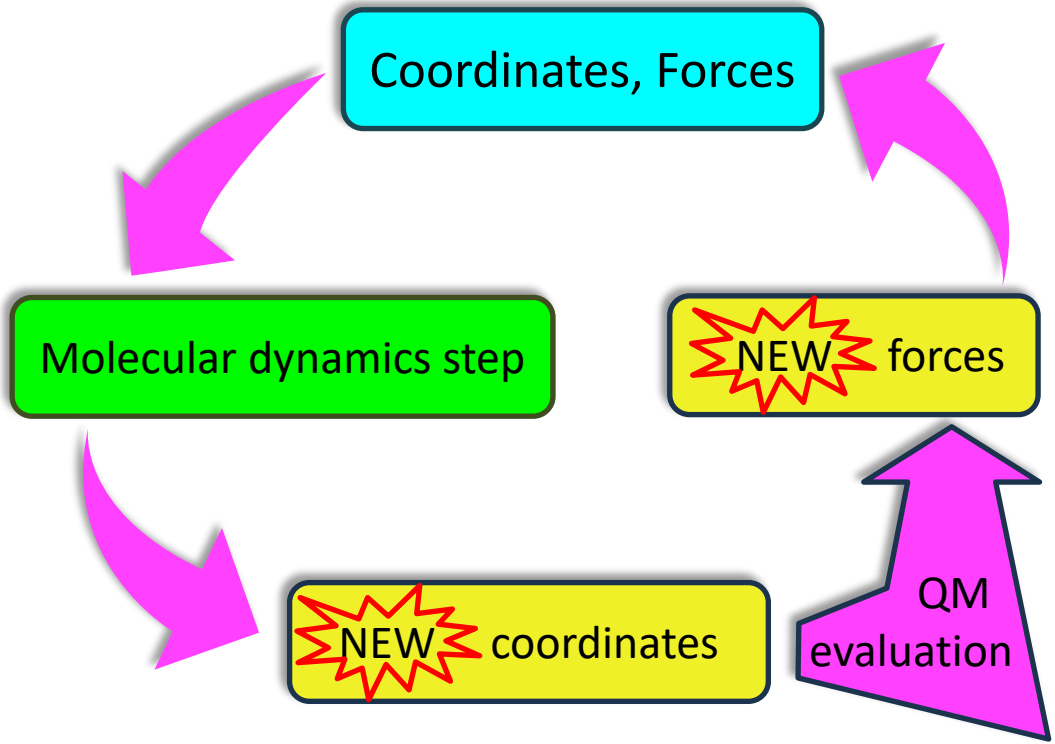
And more in the manual...





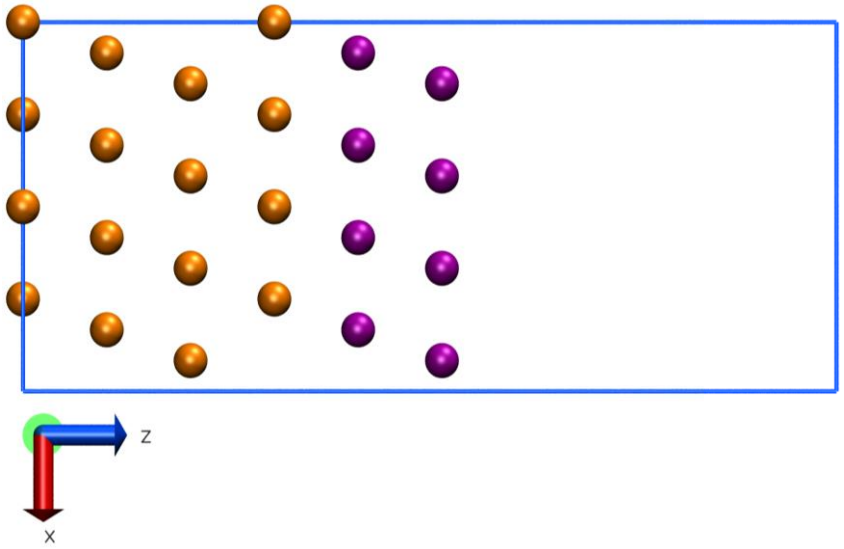
Changes in the input file

More options in the manual

- Set runtype to MD:
  - ***MD.TypeOfRun*** Verlet, Nose, …
- Set the initial time step:
  - ***MD.InitialTimeStep*** 1
- Set the final time step:
  - ***MD.FinalTimeStep*** 100
- Set the time step:
  - ***MD.LengthTimeStep*** 1 fs
- Set temperature/pressure
  - ***MD.TargetTemperature*** 300 K

Use of constraints

When relevant, one can constrain the movement of atoms




```
%block GeometryConstraints
atom Cu
%endblock GeometryConstraints

or

%block GeometryConstraints
position from 1 to 48
%endblock GeometryConstraints
```

How to continue calculations not finished?

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Both geometry optimization and molecular dynamics allow for that

- Files that can be read:
  - ***SystemLabel.XV*** (vel. and coord.)
  - ***SystemLabel.X_RESTART***
    - X is the type of MD
- Manually:
  - Insert the last coordinates;
  - For MD, initial velocities will be generated in this case.
- The ***SystemLabel.{ANI,MDE}*** will be updated

Make sure files will be read

- ***MD.UseSaveXV*** **true**

Controlling output data

Not everything is printed by default…

- Mulliken charges:
  - ***WriteMullikenPop*** 1
- Charges for MD:
  - ***PartialChargesAtEveryGeometry*** true
- Electrostatic potential:
  - ***SaveElectrostaticPotential*** true
- Total potential:
  - ***SaveTotalPotential*** true
- Coordinate steps:
  - ***WriteCoorStep*** true

How to post-process data?

Types of post-processing that can be done

- Files:
  - ***SystemLabel.MDE***
    - ***Temperature, energy…***
  - ***SystemLabel.out***
    - ***Grep command can be used to extract information to be plotted.***

To plot directly on the terminal

Executable

plot_md.sh

To plot the energies:

plot_md.sh SystemLabel.MDE 1 2 #will plot the first and second columns of the MDE file

To plot the energies from a grep command:

grep enth | plot_md.sh '<cat' 1 4 #will plot the first and fourth columns of the grep outcome

If you want to define ranges:

plot_md.sh SystemLabel.MDE 1 2 5 10 #from step 5 to 10

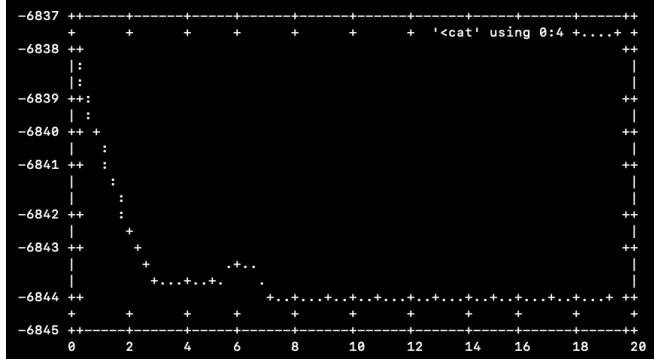
How to post-process data?

Types of post-processing that can be done

Executable

plot_md.sh

```
nct01147@login2:~/structure-optimization/work-files/SiH> grep enth sih.out
Target enthalpy (eV/cell)    -6837.8321
Target enthalpy (eV/cell)    -6840.0775
Target enthalpy (eV/cell)    -6842.3403
Target enthalpy (eV/cell)    -6843.6833
Target enthalpy (eV/cell)    -6843.5560
Target enthalpy (eV/cell)    -6843.7513
Target enthalpy (eV/cell)    -6843.4228
Target enthalpy (eV/cell)    -6844.0485
Target enthalpy (eV/cell)    -6844.0049
Target enthalpy (eV/cell)    -6844.0985
Target enthalpy (eV/cell)    -6844.1035
Target enthalpy (eV/cell)    -6844.1169
Target enthalpy (eV/cell)    -6844.1208
Target enthalpy (eV/cell)    -6844.1220
Target enthalpy (eV/cell)    -6844.1253
Target enthalpy (eV/cell)    -6844.1175
Target enthalpy (eV/cell)    -6844.1253
Target enthalpy (eV/cell)    -6844.1263
Target enthalpy (eV/cell)    -6844.1268
Target enthalpy (eV/cell)    -6844.1279
nct01147@login2:~/structure-optimization/work-files/SiH> grep enth sih.out | plot_md.sh '<cat' 0 4
```




```
nct01147@login2:~/structure-optimization/work-files/SiH>
```

How to visualize trajectories?

Files that can be used for that

- Files:
  - *SystemLabel.ANI*
    - *Coordinates trajectory.*
  - *SystemLabel.STRUCT_OUT*
    - *Last coordinates;*
    - *Need to be converted into PDB:*
      - *ASE, for instance.*

<ase convert SystemLabel.STRUCT_OUT SystemLabel.pdb>

VMD Visual Molecular Dynamics

vmd -xyz SystemLabel.ANI
vmd SystemLabel.pdb

Hands-on now

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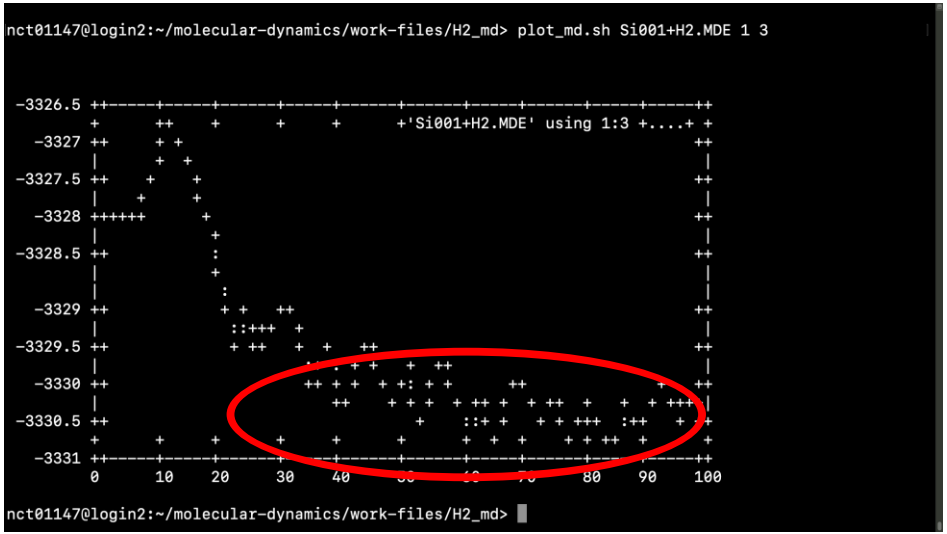
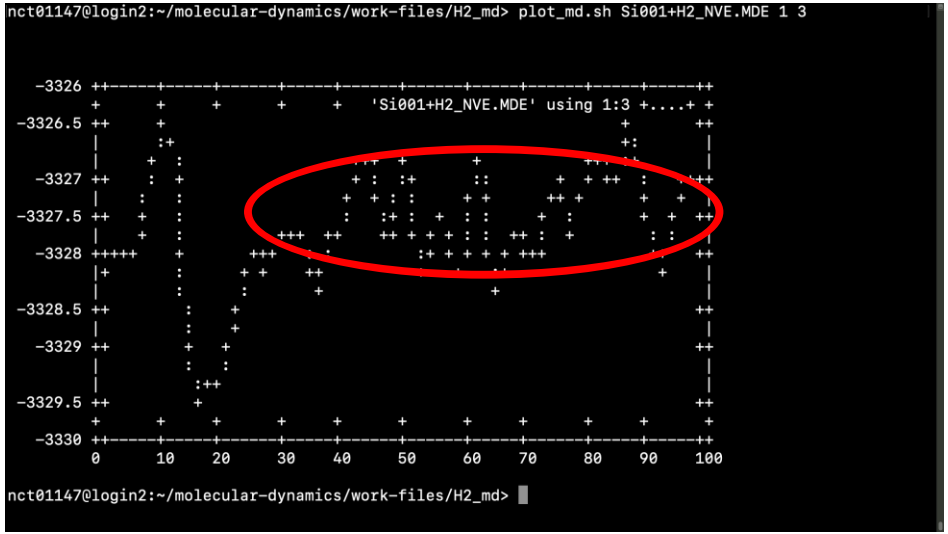
Let's try the tutorials! Questions before?

/leonardo_work/EUHPC_TD02_030/siesta-tutorials/day4-Thu/01-MolecularDynamics

Some outcomes

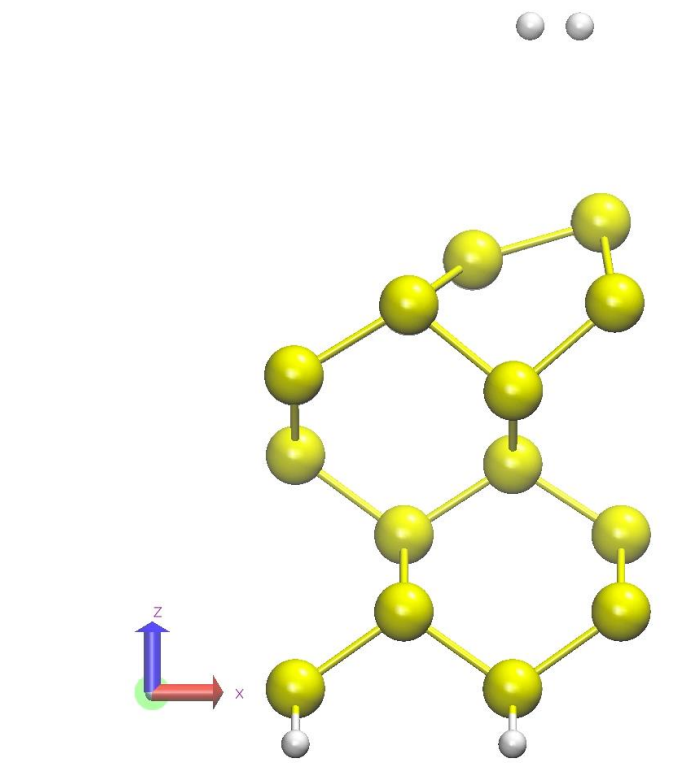
Examples of analysis that could be done

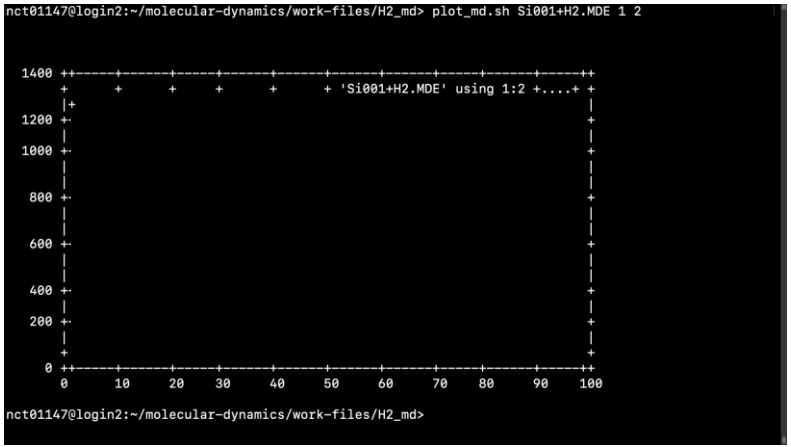


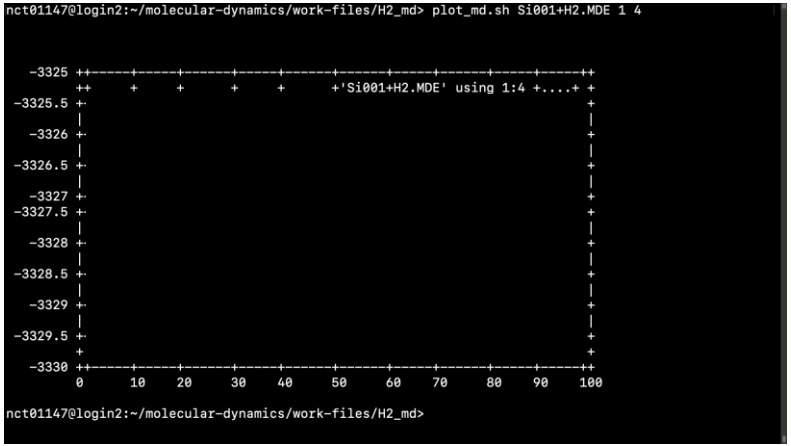


Some outcomes

Examples of analysis that could be done







The end

That's it!