chemview Documentation

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chemview is an interactive molecular viewer designed for the IPython notebook. With chemview you can:

- **Display** molecules and systems in an easy and efficient manner.
- Look at those systems evolve in **time**. chemview is fast by design, updates on the properties are performed only when necessary.
- Perform interactive data visualization in the IPython notebook.
- Create new ways to visualize your data by using the flexible low-level API.

chemview is implemented using web technologies such as WebGL and three.js, giving chemview an **excellent multi-platform support**.

Excited? Try it out (it works on smartphones too):

- Left Click: Rotate
- Wheel: Zoom
- Right Click: Pan

Go ahead with the *Installation and Quick Start*.

Contents:

CHAPTER 1

Installation and Quick Start

Installing chemview with conda is fairly easy. First download anaconda (or miniconda):

http://continuum.io/downloads

To install chemview using conda you can first create an environment (optional):

```
$ conda create -p /path/to/new/environment python
$ source activate /path/to/new/environment
```

then, you can install chemview directly from the binstar channel.

```
$ conda install -c http://conda.binstar.org/gabrielelanaro
```

or, for the development version you can manually install the dependencies:

```
$ conda install notebook numpy numba
$ git clone https://github.com/gabrielelanaro/chemview
$ cd chemview
$ pip install .
```

It is also possible to install chemview using pip:

```
pip install notebook numpy numba # Jupyter 4.x

# Download and install chemview
git clone https://github.com/gabrielelanaro/chemview
cd chemview
pip install .
```

Chemview has an optional <povray http://www.povray.org/>_ backend for rendering high quality images. For this you'll need to install the povray software and the vapory bindings:

```
pip install vapory
```

1.1 Quick Start

In this section we'll see how to visualize a benzene molecule with chemview. To start, let's launch IPython notebook and start a new notebook.

To import chemview you can write and execute the following code in a cell:

```
from chemview import MolecularViewer
```

The function enable_notebook will load the necessary files to display the molecular viewer in the browser. To display a benzene molecule we need at least two pieces of information:

1. The atomic types
2. The atomic coordinates
3. The bonds between atoms

For the scope of this tutorial, the information were extracted from here. You can use chemical package (like mdtraj or chemlab) to read the coordinates of your molecules.

We define the coordinates as a numpy array, the atomic types as a list of strings and the bonds as a list of start, end tuples.

```
import numpy as np
coordinates = np.array([[0.00, 0.13, 0.00], [0.12, 0.07, 0.00], [0.12,-0.07, 0.00],
                        [0.00,-0.14, 0.00], [-0.12,-0.07, 0.00],[-0.12, 0.07, 0.00],
                        [ 0.00, 0.24, 0.00], [ 0.21, 0.12, 0.00], [ 0.21,-0.12, 0.00],
                        [ 0.00,-0.24, 0.00], [-0.21,-0.12, 0.00],[-0.21, 0.12, 0.00]])
atomic_types = ['C', 'C', 'C', 'C', 'C', 'C', 'H', 'H', 'H', 'H', 'H', 'H']
bonds = [(0, 6), (1, 7), (2, 8), (3, 9), (4, 10), (5, 11),
         (0, 1), (1, 2), (2, 3), (3, 4), (4, 5), (5, 0)]
```

We can pass those to the class MolecularViewer and call the method lines to render the molecule as a wireframe:

```
mv = MolecularViewer(coordinates, topology={'atom_types': atomic_types,
                                             'bonds': bonds})
mv.lines()
mv
```

You can rotate (left click), pan(right click) and zoom (wheel) to visualize your molecules.

Congratulation for finishing the first tutorial! You can now move on more advanced topics:

1.1.1 Viewing Molecules

Using the MolecularViewer

MolecularViewer is a library-agnostic tool to display molecules in chemview. In this section we will see how to use it, and what representations are currently available.

To create a MolecularViewer instance we need the **positions** of the atoms, as an array of x, y, z coordinates, and a description of the features and connectivity of the system (also called **topology**).

The *topology* is a nested dictionary with the following fields:

atom_types (required field) A list of strings, each representing an atom symbol.

Example: `["H", "C", "N", "O", ..]`

bonds A list of tuples indicating the index of the bond extrema.

Example: `[(0, 1), (1, 2), ...]`

atom_names A list of atom names, like the ones used in pdb files

Example: `["HA", "CA", "N", ...]`

residue_indices A nested list of indices (as tuples) for each residue present in the molecule.

Example: `[(0, 1, 2, 3, 4, 5), (6, 7, 8, 9, 10), ... ]`

residue_types A list of strings corresponding to residue types.

Example: `["ALA", "GLY", ...]`

secondary_structure A list of strings representing the secondary structure of each residue, `H` for helix, `E` for sheet, `C` for coil.

Example: `["H", "H", "H", "C", "C", "E", "E" ...]`

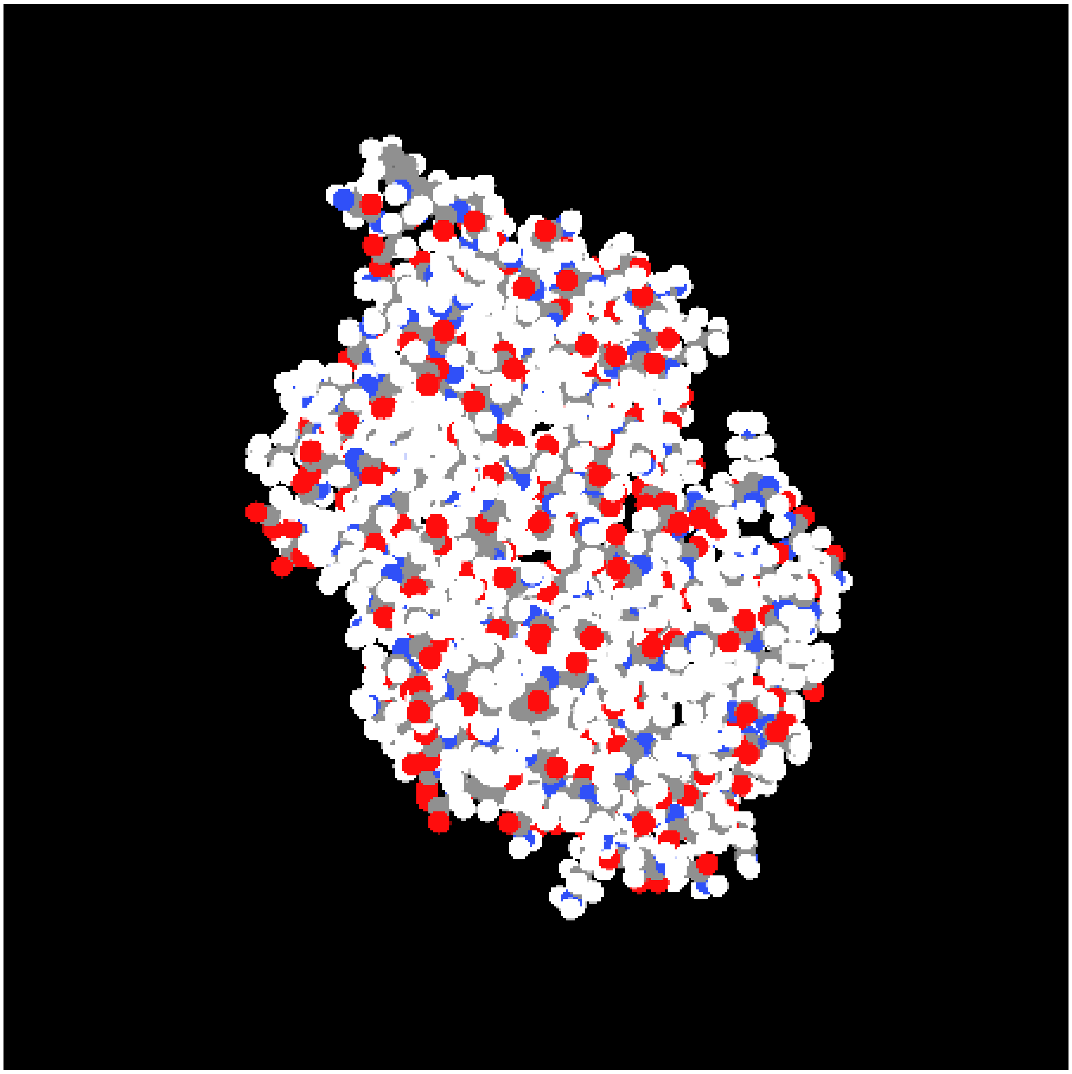
Note: As the description of the topology is quite involved, you can combine chemview with another library that provides the topology directly from the chemical data files (such as chemlab and mdtraj).

Once you create your molecular viewer, you can display the molecule in a variety of ways:

- points: the atomic positions will be represented as points, color-coded by atom.

  Example:

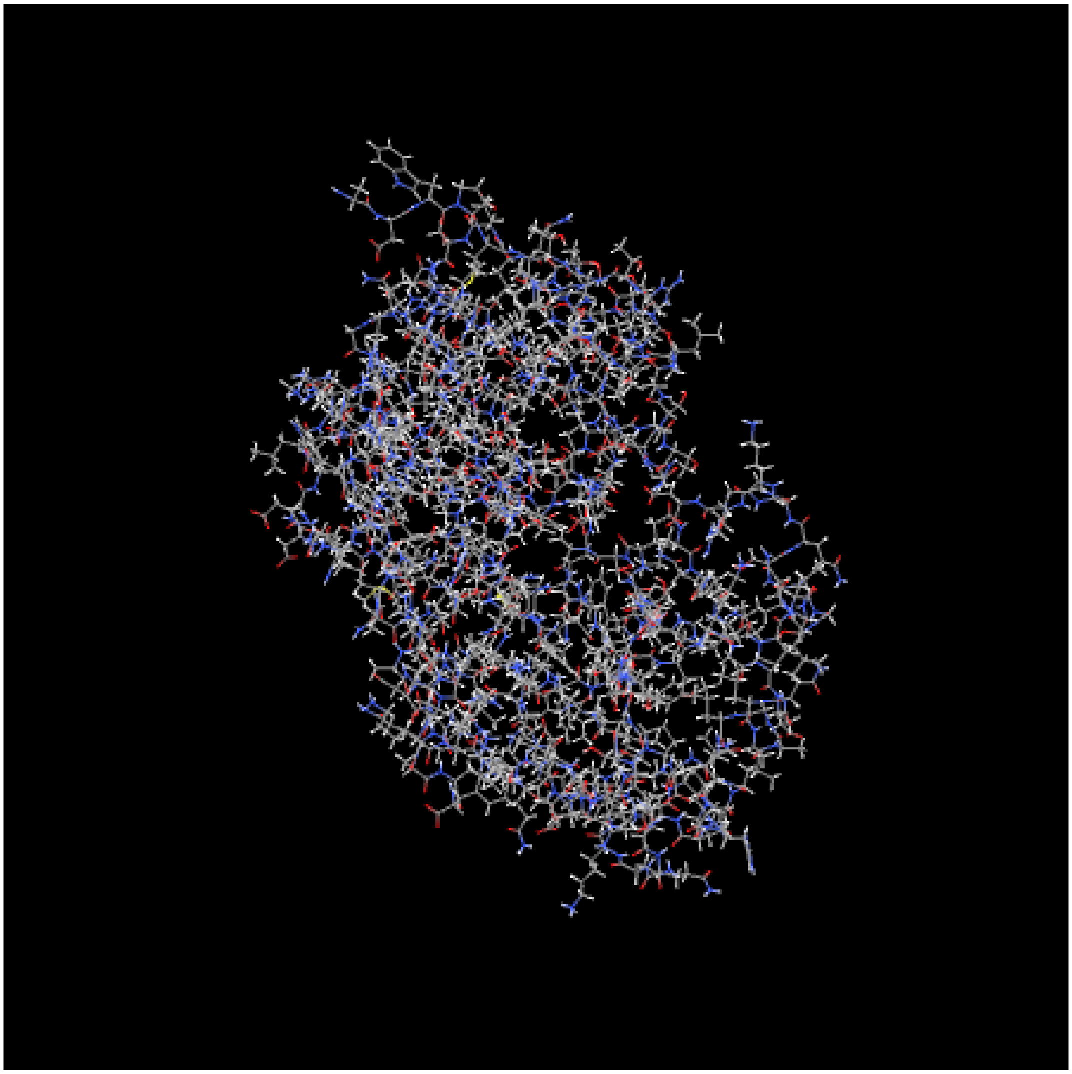
  ```
  mv.points()
  ```



- lines: the bonds will be represented as lines

  Example:

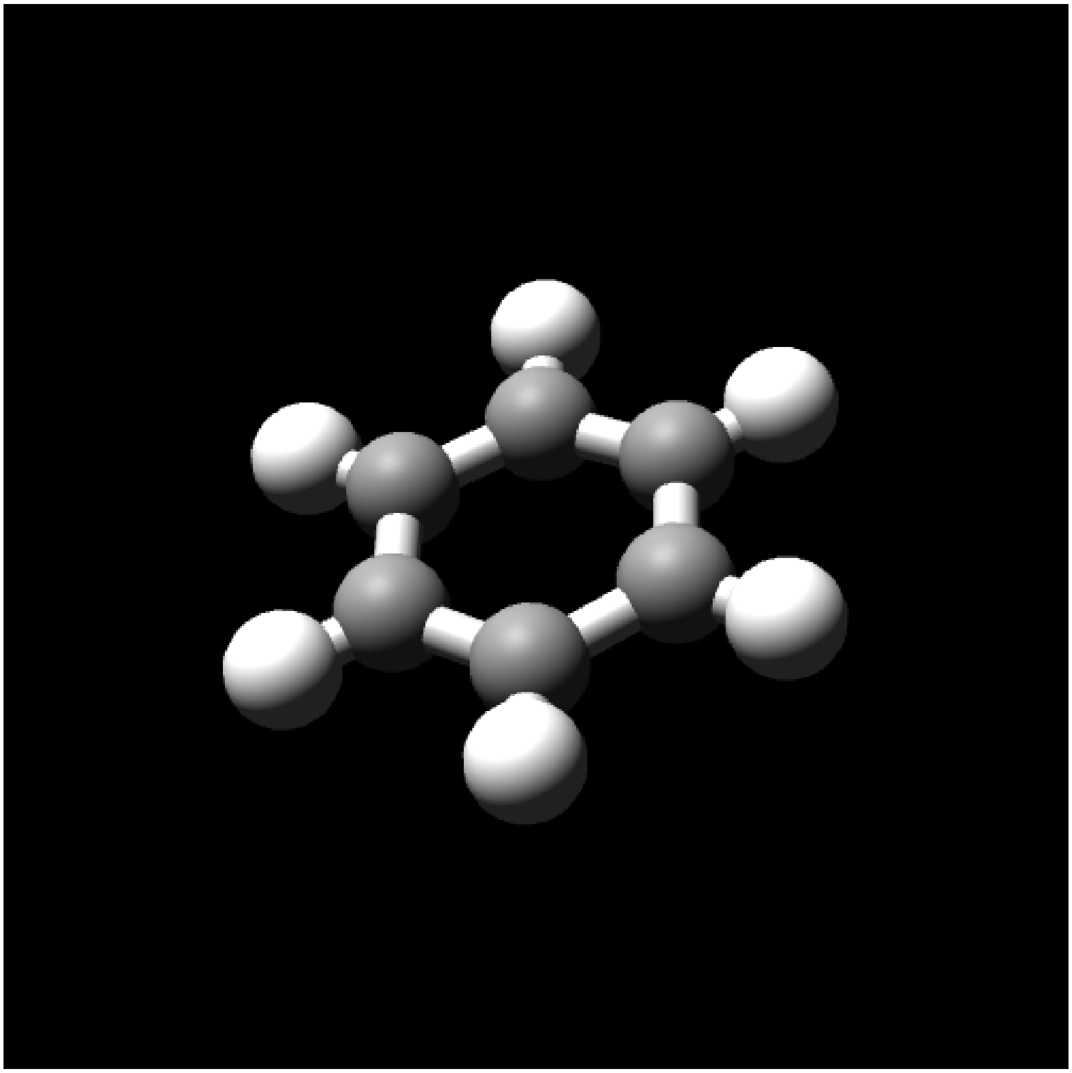
  ```
  mv.lines()
  ```



- ball_and_sticks: the classical ball and stick representation. Atom are spheres, bonds are cylinders. At the moment this representation is not suitable for very large molecules and animations.

  Example:

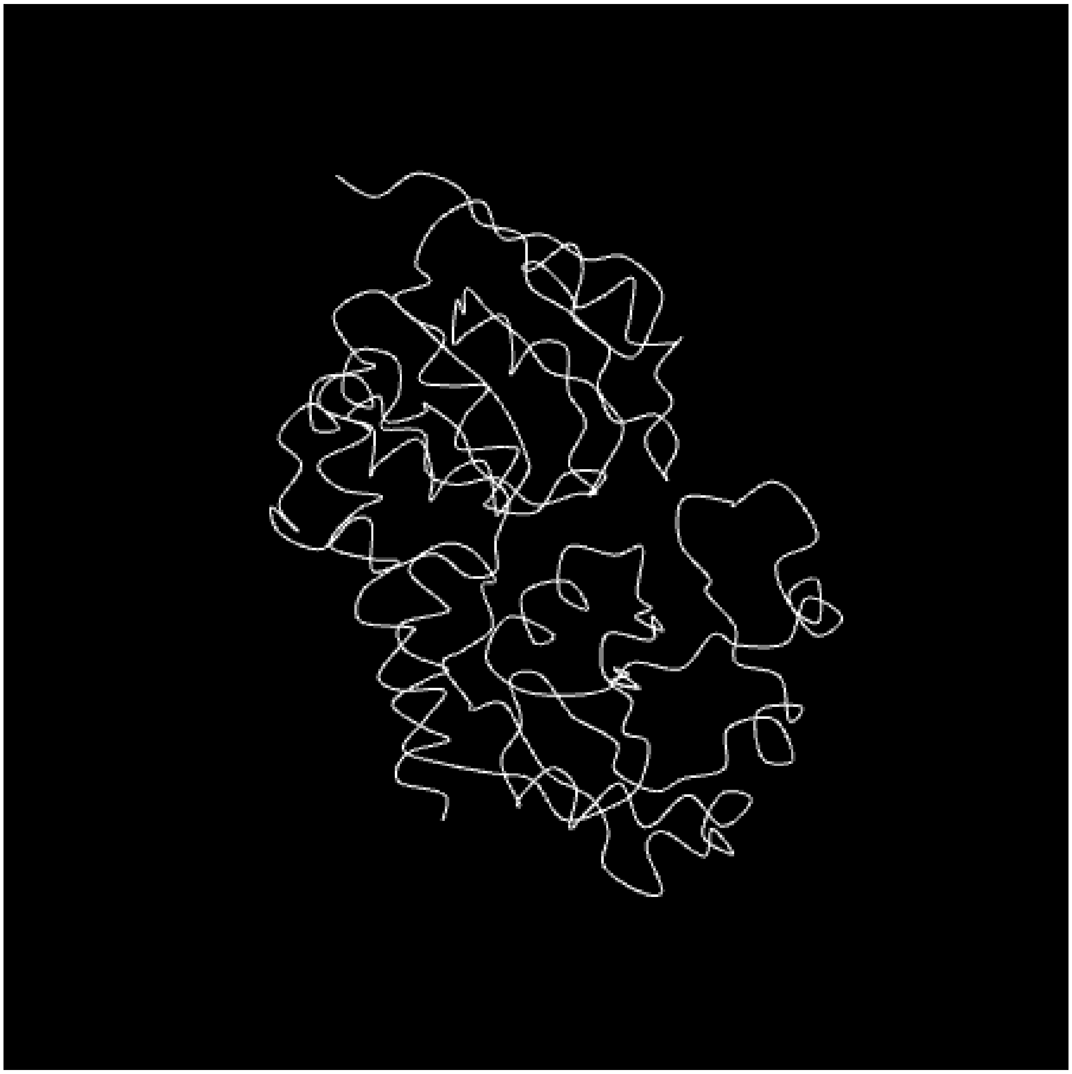
  ```
  mv.ball_and_sticks()
  ```



- line_ribbon: the protein backbone is represented by a smooth line.

  Example:

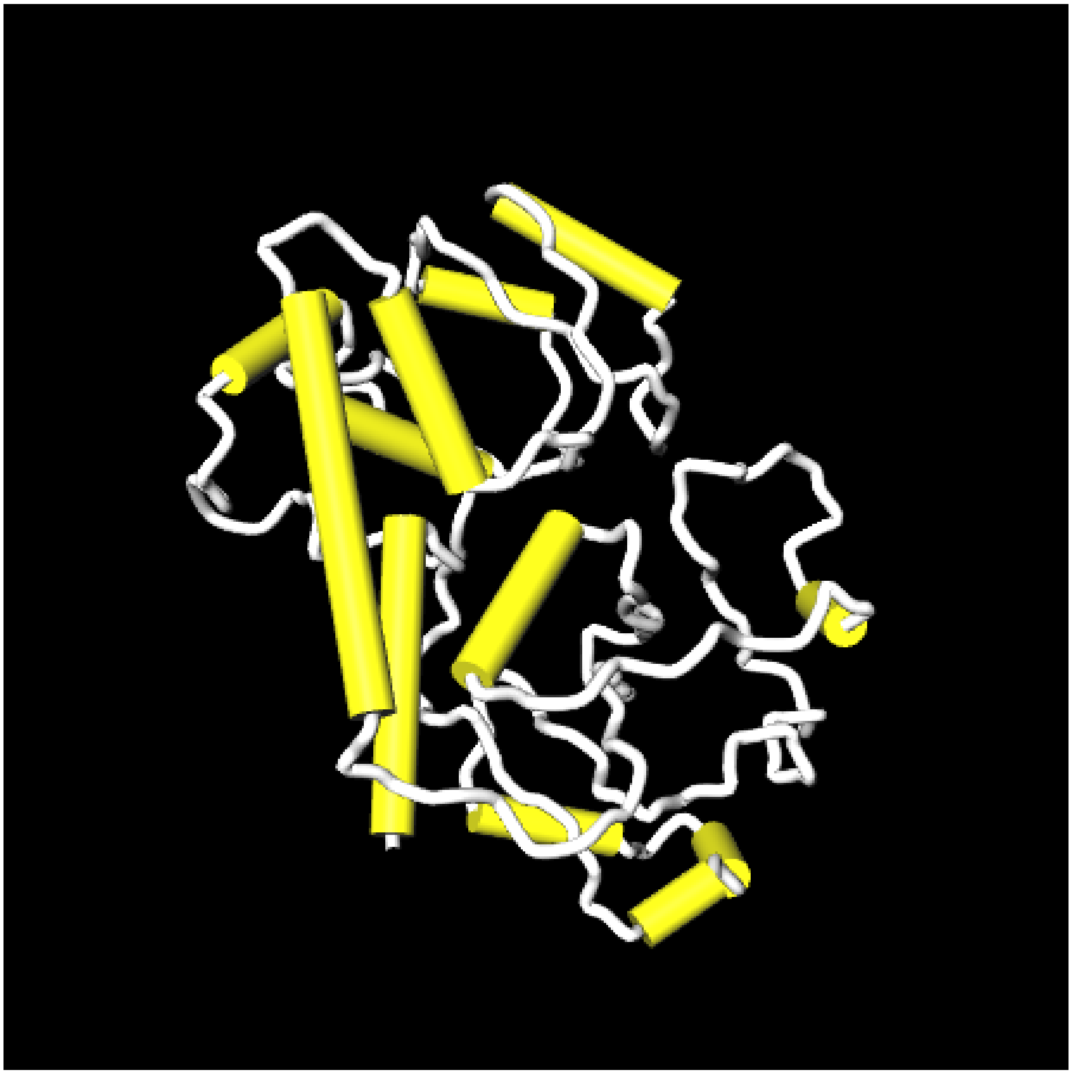
  ```
  mv.line_ribbon()
  ```



- cylinder_and_strand: the protein backbone is represented by a smooth, solid tube, and the helices are represented as cylinders.

  Example:

  ```
  mv.line_ribbon()
  ```



See also:

The `MolecularViewer` documentation at api/index

You can also add isosurfaces with the command `MolecularViewer.add_isosurface()` that takes a function and an isovalue. Given a function $f(x, y, z)$, an isosurface is the set of points for which the function assumes a certain value. For example if you want to plot the surface of sphere with radius 1, we can select a function of the type:

$$f(x, y, z) = x^2 + y^2 + z^2$$

and set the isovalue would be 1, so that we obtain the surface whose set of points that satisfy the equation of a sphere:

$$x^2 + y^2 + z^2 = 1$$

See also:

Plotting molecular orbitals

Viewing Molecules with Chemlab

The development version of chemlab provides a preliminary integration with chemview, check out the example notebook.

Viewing Molecules with MDTraj

In the near future, mdtraj will provide integration.

While you wait, take a look at the docs and learn about mdtraj.

Making custom representations

chemview provides an easy-to-use API to create new ways to display your data and build novel tools. The class RepresentationViewer contains methods to display common 3D shapes.

To create a RepresentationViewer instance, type:

```
rv = RepresentationViewer()
rv
```

This will display an empty viewer. To add objects, we can use the method *`RepresentationViewer.add_representation()`*. The method takes two parameters: the **name** of the representation to display, and a dictionary of **options**, that are specific for each representation.

For example, to add three points on the screen we will use the following parameters:

```
rv.add_representation('points', {'coordinates', np.array([[0.0, 0.0, 0.0],
                                                           1.0, 0.0, 0.0],
                                                           2.0, 0.0, 0.0])})
```

> **Warning:** The RepresentationViewer communicates directly with the Javascript layer and, being outside of the realm of Python doesn't provide nice exception tracebacks. Be rigorous with parameter types.

For more examples (with pictures) you can check the test notebook.

Below reference of the available representations, along with their options:

points display a set of coordinates as points with different colors and sizes.

Options:

- **coordinates** numpy array of 3D coordinates (float32)
- **sizes** python list of floats representing the size of each point
- **colors** python list of 32 bit integers representing the color of each point.

  Example using HEX representation: `[0xffffff, 0x00ffff, 0xff0000, ...]`

lines display a set of lines with different colors.

Options:

- **startCoords** numpy array of 3D coordinates representing the starting point of each line
- **endCoords** numpy array of 3D coordinates representing the ending point of each line
- **startColors** list of 32 bit integers corresponding to the color of the starting point
- **endColors** list of 32 bit integers corresponding to the color of the ending point

cylinders display a set of cylinders. This is a slow primitive, avoid using it for animations; use *lines* instead.

Options:

- **startCoords** numpy array of 3D coordinates representing the starting point of each cylinder

- **endCoords** numpy array of 3D coordinates representing the ending point of each cylinder
- **colors** list of 32 bit integers corresponding to the color of each cylinder
- **radii** list of float corresponding to the radius of each cylinder

smoothline display a smooth line that passes through a set of points.

Options:

- **coordinates** numpy array of 3D coordinates representing the *control points* of the smooth line.
- **color** 32 bit integer (hex) color of the line
- **resolution** int, number of subdivision along the path between control points. Controls the *smoothness*

smoothtube display a smooth tube that passes through a set of points. This is a slow primitive, not suitable for animating very large objects; use *smoothline* instead.

Options:

- **coordinates** numpy array of 3D coordinates representing the *control points* of the smooth tube.
- **color** 32 bit integer (hex) color of the tube
- **radius** float representing the radius of the tube
- **resolution** int, number of subdivision along the path between control points. Controls the *smoothness*

spheres display a set of spheres. This primitive is slow, avoid using it for animations; use *points* instead.

Options:

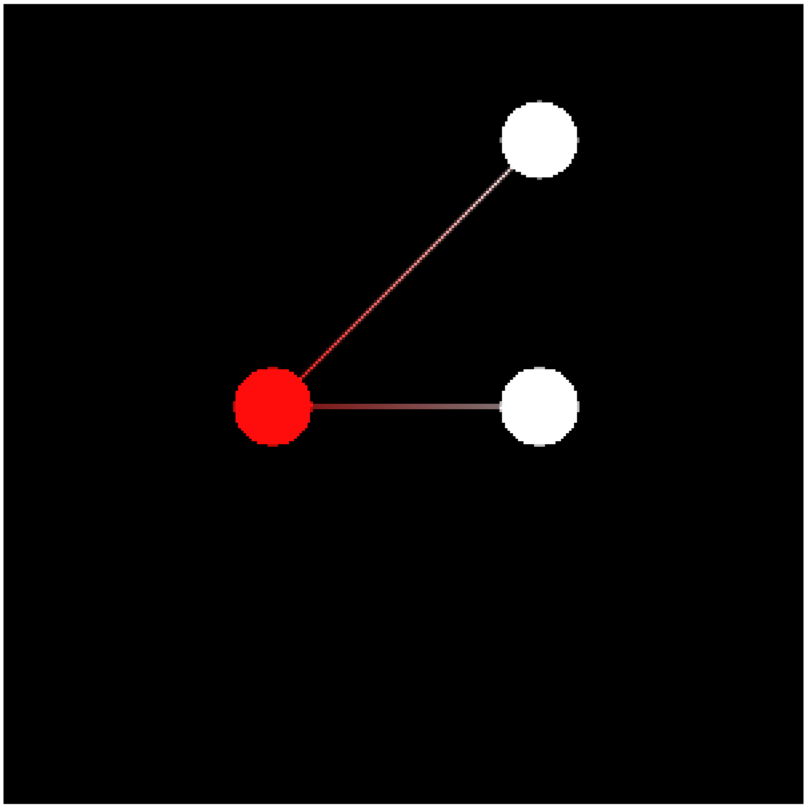
- **coordinates** numpy array of 3D coordinates representing the position of the spheres.
- **colors** list of 32 bit integers representing the color of each sphere
- **radii** list of float, radius of each sphere
- **resolution** int, number of vertical and horizontal subdivisions to make the sphere: high resolution means slow performance.

1.1.2 Animation

In this section we'll see how to update the molecular viewer. We'll start by creating a water molecule using the `MolecularViewer`:

```
import numpy as np
from chemview import MolecularViewer

# Draw a water molecule
mv = MolecularViewer(np.array([[0.0, 0.0, 0.0], [1.0, 0.0, 0.0], [0.0, 1.0, 0.0]]),
                     {'atom_types': ['H', 'O', 'H'],
                      'bonds': [[0, 1], [1, 2]]},
                     width = 300,
                     height = 300)
mv.points()
mv.lines()
mv
```



then, all we need to do to move the molecule is to assign a new vector to the attribute `coordinates`. To translate the molecule, we add 0.1 to the x coordinate of each atom:

```
new_coordinates = mv.coordinates + [0.1, 0.0, 0.0]
mv.coordinates = new_coordinates
```

Important: To properly update the coordinates, you have to the = (equal) sign, or the system won't detect the update. Example:

```
# Good: update will be triggered
mv.coordinates = mv.coordinates + [0.1, 0.0, 0.0]

# Bad: update won't be triggered
mv.coordinates += [0.1, 0.0, 0.0]
```

Visualizing Trajectories/Frames

Chemview can display snapshots of systems evolving in time, using a video-player like interface. This functionality is provided by the TrajectoryViewer class. The TrajectoryViewer widget is a combination of a `MolecularViewer` widget and a set of controls that automatically update the frames.

To start, we'll see expand of the previous example. To use the `TrajectoryViewer`, we need a list of coordinates (one for each frame), and the topology. We first create the initial frame *start_coordinates*, then we translate those coordinates by 0.1 units in the x axis for 30 times, once for each frame:

```
start_coordinates = np.array([[0.0, 0.0, 0.0], [1.0, 0.0, 0.0], [0.0, 1.0, 0.0]])
```

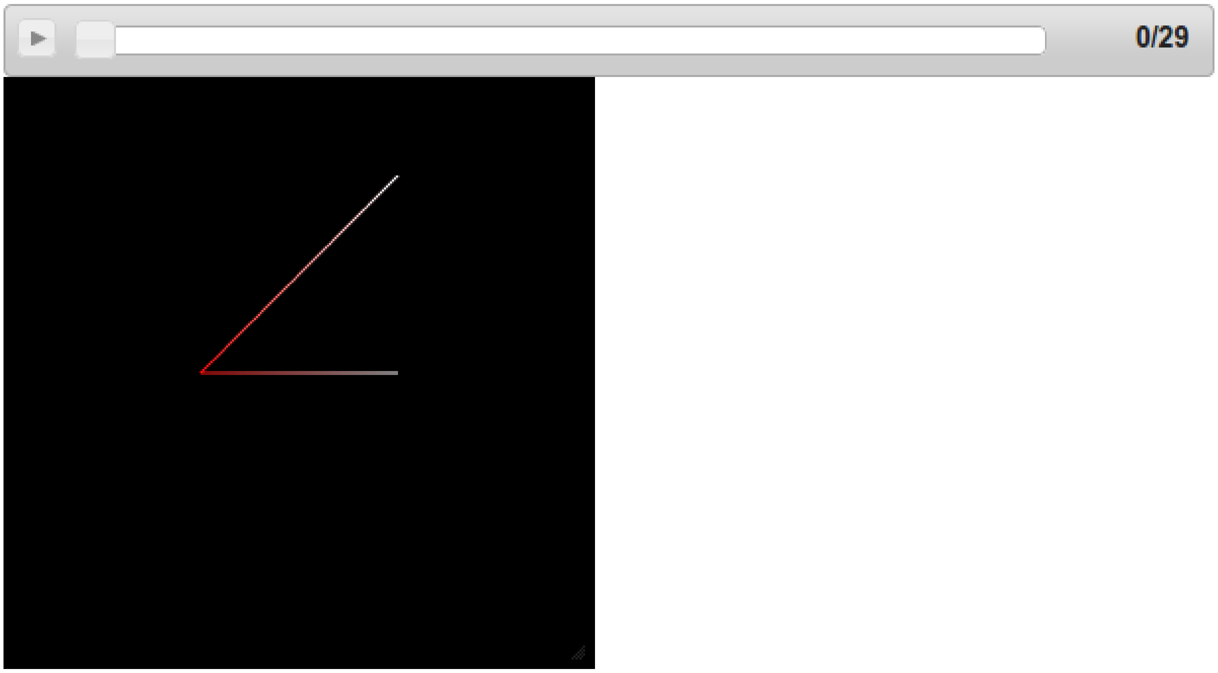
```
frames = []
for i in range(30):
    frames.append(start_coordinates + [0.1, 0.0, 0.0])
    start_coordinates += [0.1, 0.0, 0.0]
```

At this point, we can use the trajectory viewer to visualize the frames.

```
from chemview import TrajectoryViewer

tv = TrajectoryViewer(frames, {'atom_types': ['H', 'O', 'H'],
                               'bonds': [[0, 1], [1, 2]]})
tv.lines()
tv
```

Screenshot:



You should now have a nice bar that lets you play, pause, rewind your frames!

Using mdtraj

How do we use the trajectory viewer in practice? To show a real-world example we can get some help from the library mdtraj.

With mdtraj we can read a system and a series of snapshots generated from a simulation.

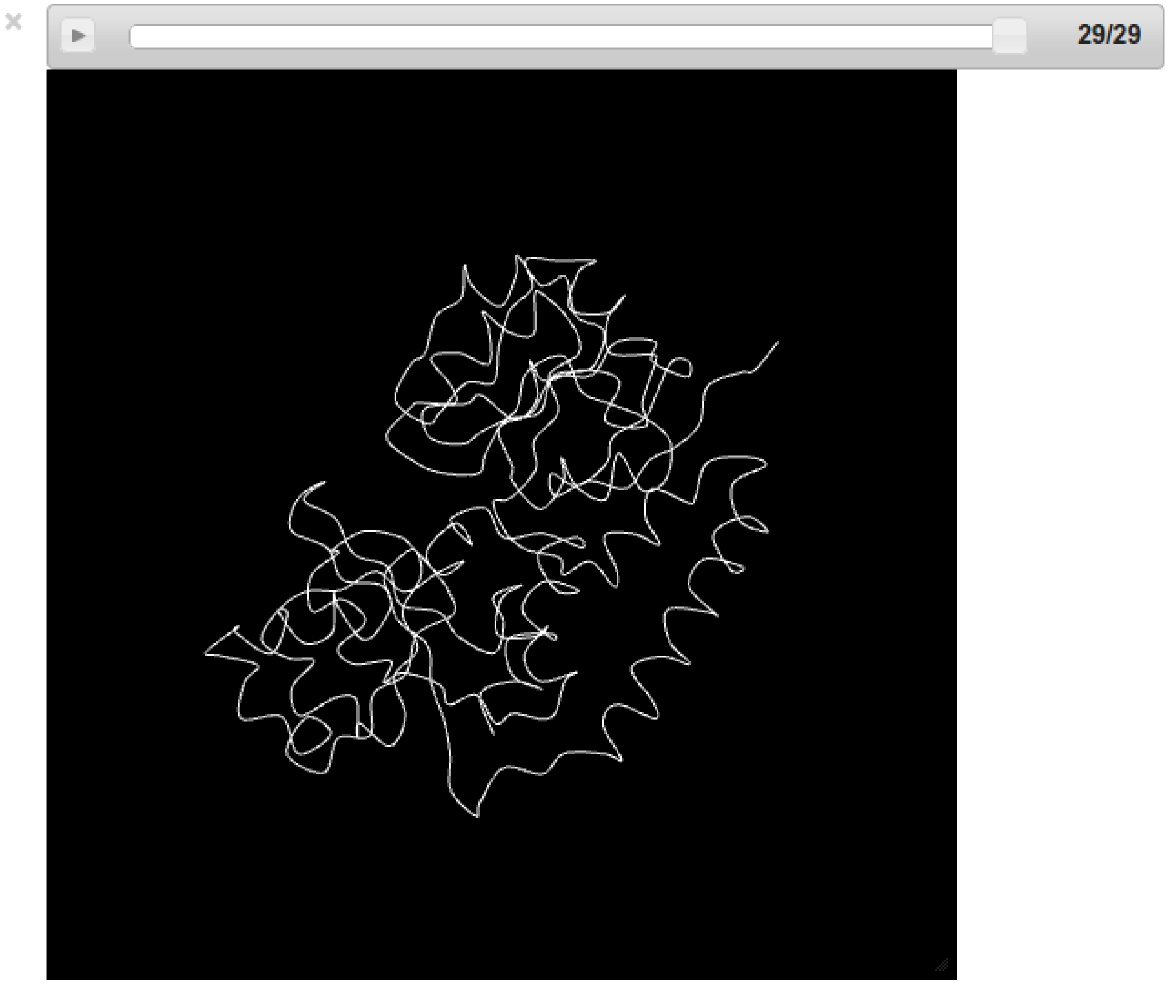
```
import mdtraj as md
traj = md.load_pdb('2M6K.pdb')
```

An mdtraj trajectory contains the coordinates for each frame in the attribute `traj.xyz`), plus a topology specification in `traj.topology`. The topology can be converted to chemview format using the utility `chemview.contrib.topology_mdtraj()`, that takes the trajectory as an input.

```
from chemview.contrib import topology_mdtraj

tv = TrajectoryViewer(traj.xyz, topology_mdtraj(traj))
tv.line_ribbon()
tv
```

Screenshot:



Tip: When animating trajectories of big molecules and systems, use simple representations such as `lines`, `points` and `line_ribbon` because they are much faster than their "solid" counterparts `vdw`, `ball_and_stick` and `strand`.

1.1.3 Low Level API

API Reference

Module `chemview.widget`

class RepresentationViewer(*self*, *width=500*, *height=500*)

RepresentationViewer is an IPython notebook widget useful to display 3d scenes through webgl.

Example:

```
from IPython.display import display

rv = RepresentationViewer()
rv.add_representation('point', {'coordinates': coordinates, 'colors': colors,
↪'sizes': sizes})
display(rv)
```

add_representation(*self*, *rep_type*, *options*)

Add a 3D representation to the viewer. See User Guide for a complete description of the representations available.

Returns An unique hexadecimal identifier for the representation.

Return type str

remove_representation(*self*, *rep_id*)

Remove a representation from the viewer

Parameters **rep_id** (*str*) – the unique identifier generated by RepresentationViewer.add_representation

update_representation(*self*, *rep_id*, *options*)

Update a representation with new data.

Parameters

- **rep_id** (*str*) – the unique identifier returned by RepresentationViewer.add_representation
- **options** (*dict*) – dictionary containing the updated data.

class TrajectoryControls(*self*, *n_frames*, *fps=30*)

Play/Pause controls useful for playing trajectories.

Example:

You can connect a callback to be executed every time the frame changes.

```
from IPython.display import display

controls = TrajectoryControls(10) # 10 frames

def callback(frame):
    print("Current frame %d" % frame)

controls.on_frame_change(callback)
display(controls)
```

frame

Current frame

n_frames
Total number of frames

fps
Frames per second (defaults to 30)

on_frame_change (*self*, *callback*)
Connect a callback to be executed every time the frame attribute changes.

Module `chemview.viewer`

class MolecularViewer (*self*, *coordinates*, *topology*, *width=500*, *height=500*)
Create a Molecular Viewer widget to be displayed in IPython notebook.

Parameters

- **coordinates** (*np.ndarray*) – A numpy array containing the 3D coordinates of the atoms to be displayed
- **topology** (*dict*) – A dict specifying the topology as described in the User Guide.

points (*self*, *size=1.0*)
Display the system as points.

Parameters **size** (*float*) – the size of the points.

lines (*self*)
Display the system bonds as lines.

wireframe (*self*, *pointsize=0.2*)
Display atoms as points of size *pointsize* and bonds as lines.

ball_and_sticks (*self*, *ball_radius=0.05*, *stick_radius=0.02*)
Display the system using a ball and stick representation.

line_ribbon (*self*)
Display the protein secondary structure as a white lines that passes through the backbone chain.

cylinder_and_strand (*self*)
Display the protein secondary structure as a white, solid tube and the alpha-helices as yellow cylinders.

add_isosurface (*self*, *function*, *isolevel=0.3*, *resolution=32*, *style='wireframe'*, *color=16777215*)
Add an isosurface to the current scene.

Parameters

- **function** (*callable*) – A function that takes x, y, z coordinates as input and is broadcastable using numpy. Typically simple functions that involve standard arithmetic operations and functions such as `x**2 + y**2 + z**2` or `np.exp(x**2 + y**2 + z**2)` will work. If not sure, you can first pass the function through `numpy.vectorize`. Example: `mv.add_isosurface(np.vectorize(f))`
- **isolevel** (*float*) – The value for which the function should be constant.
- **resolution** (*int*) – The number of grid point to use for the surface. An high value will give better quality but lower performance.
- **style** (*str*) – The surface style, choose between `solid`, `wireframe` and `transparent`.
- **color** (*int*) – The color given as an hexadecimal integer. Example: `0xffffff` is white.

Module `chemview.trajectory`

class TrajectoryViewer(*self*, *coordinate_frames*, *topology*, *width=500*, *height=500*)

Display a trajectory in the IPython notebook.

Parameters

- **coordinate_frames** (*list*) – A list containing the positions of the atoms (as np.ndarray) for each frame.
- **topology** (*dict*) – A dictionary specifying the topology

See also:

MolecularViewer

Module `chemview.utils`

encode_numpy(*array*)

Encode a numpy array as a base64 encoded string, to be JSON serialized.

Returns a dictionary containing the fields: - *data*: the base64 string - *type*: the array type - *shape*: the array shape

get_atom_color(*atom_name*)

CHAPTER 2

Cookbook

This documents contains *recipes* to accomplish common tasks with `chemview`.

2.1 Syncronizing cameras across multiple widgets

Using the IPython traitlets system it is possible to syncronize the camera across different widgets. In the following example we download two molecules (ethane and butane) from the web using the chemlab API, then we create two molecular viewers and we link their cameras:

```
from IPython.display import display
from IPython.utils.traitlets import link

from chemview import MolecularViewer

from chemlab.notebook import download_molecule

butane = download_molecule('butane')
ethane = download_molecule('ethane')

# Create the two molecular viewer widgets
mv1 = MolecularViewer(butane.r_array, {'atom_types': butane.type_array,
                                       'bonds': butane.bonds})
mv1.wireframe()

mv2 = MolecularViewer(ethane.r_array, {'atom_types': ethane.type_array,
                                       'butane': butane.bonds})
mv2.wireframe()

# Link their attributes camera_str together
link((mv1, 'camera_str'), (mv2, 'camera_str'))

display(mv1)
display(mv2)
```

2.2 Plotting molecular orbitals

chemview is licensed under the LGPL2 and is hosted on github at http://github.com/gabrielelanaro/chemview.

CHAPTER 3

Credits

chemview branched from the mdtraj project in an effort to make trajectory viewing possible in the browser. It is developed mainly by Gabriele Lanaro. While the code is original work, the idea was inspired by iview.

CHAPTER 4

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