

# **Get your feet wet!**

## **Introduction to the nanoHUB Simulation Environment**

**Tanya Faltens, Ph.D.**  
**Network for Computational Nanotechnology**  
**Purdue University**



# Overview

- What is nanoHUB
- Simulation Examples
  - Carbon nanostructures
  - Molecular vibrations
  - Biological molecules
- Jupyter notebooks
- The nanoHUB dashboard

# What is nanoHUB?



# An open-access cyberinfrastructure

**National Science Foundation**  
**EEC 1227110**

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation





# A library of STEM resources

A wooden toolbox filled with various tools. The toolbox is made of light-colored wood and has a black interior. The tools are organized into compartments. On the left, there are several brushes and a spray bottle. In the center, there is a blue flashlight and a red saw. On the right, there is a hammer, a level, and a roll of tape. The toolbox is placed on a wooden deck.

# A Simulation Toolbox



# A Workspace

A historical printing press workshop. In the center is a large wooden galley labeled 'CENTAUR' with a grid of type cases on top. To the right is a large black metal press labeled 'ALBION PRESS HENRY MAKER WATTS LONDON'. The room is filled with various printing equipment, including a smaller table with galleys on the left, shelves with books and boxes in the background, and a hanging lamp on the left. The walls are made of rough stone or plaster.

# A Publishing Platform





# A Scientific Community

**1.9 M annual users worldwide**

HUB usage 2016-01-01 00:00:00

Come on in,

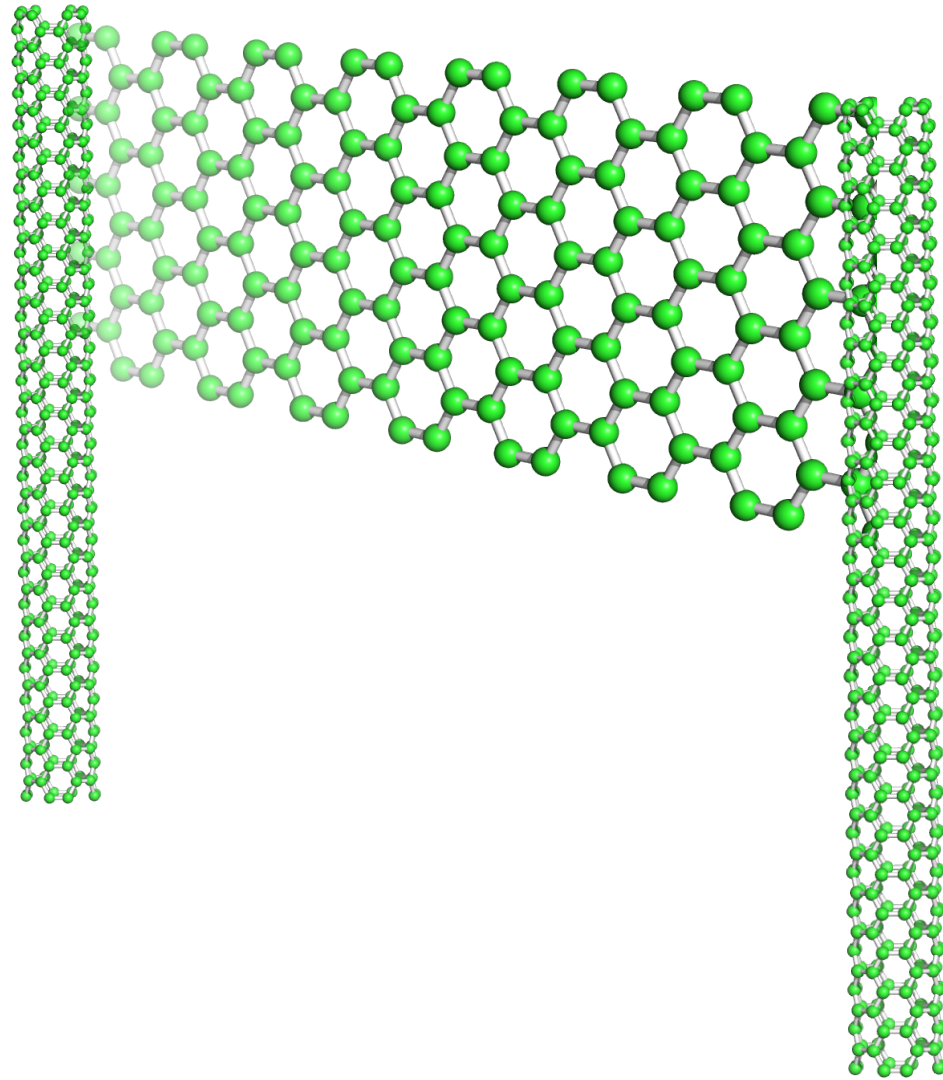
the water's fine!

# QR Code for the Handout



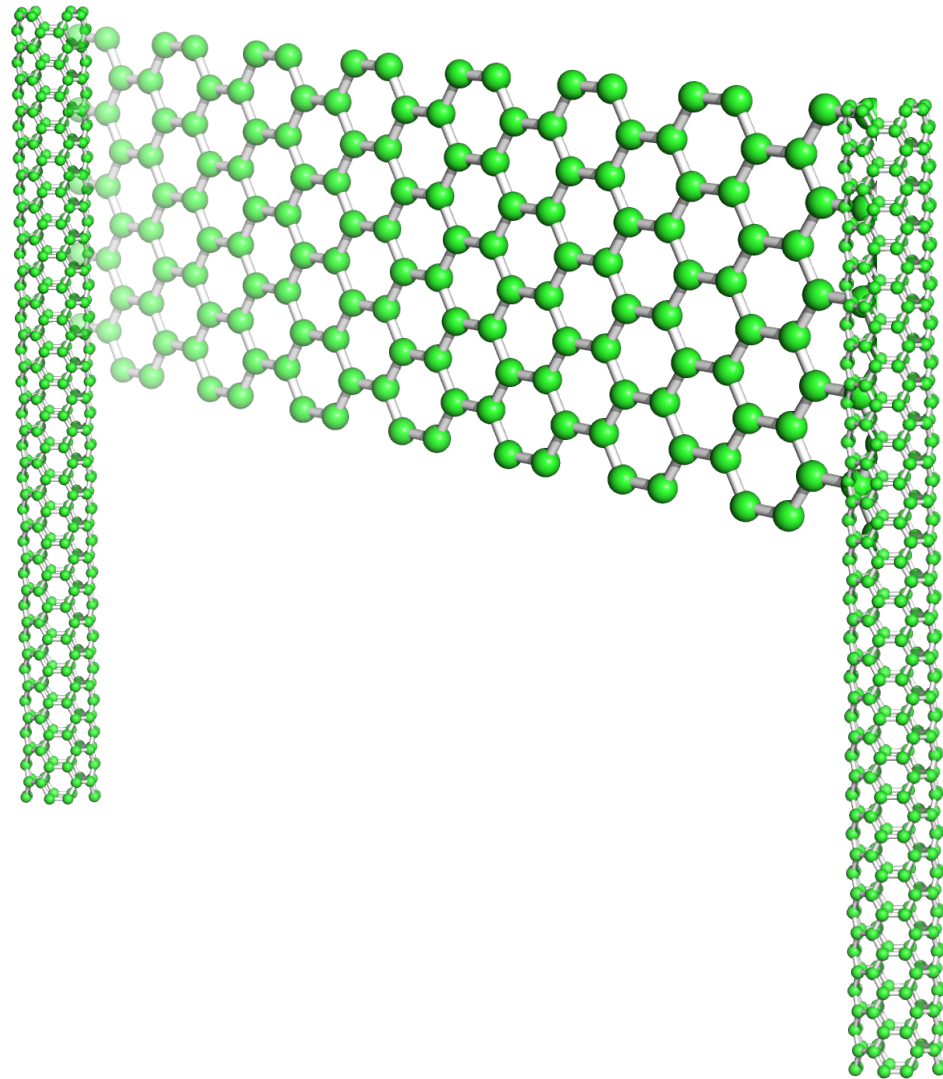
<https://tinyurl.com/nH2021Mar16>

# Fun with Carbon Nanostructures

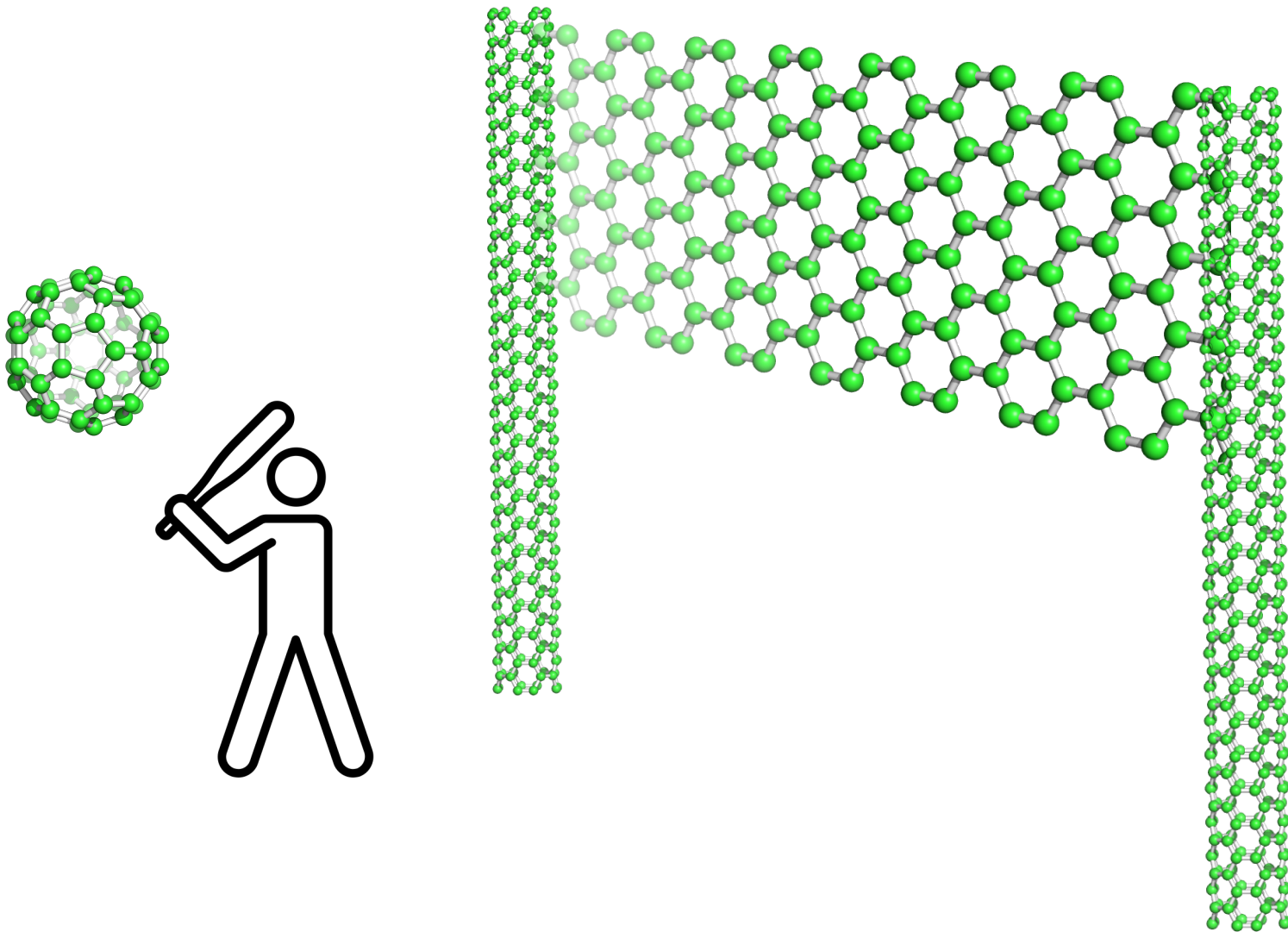


choose a player

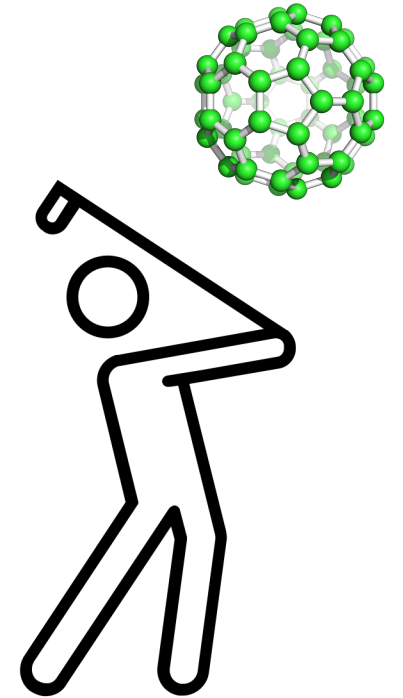
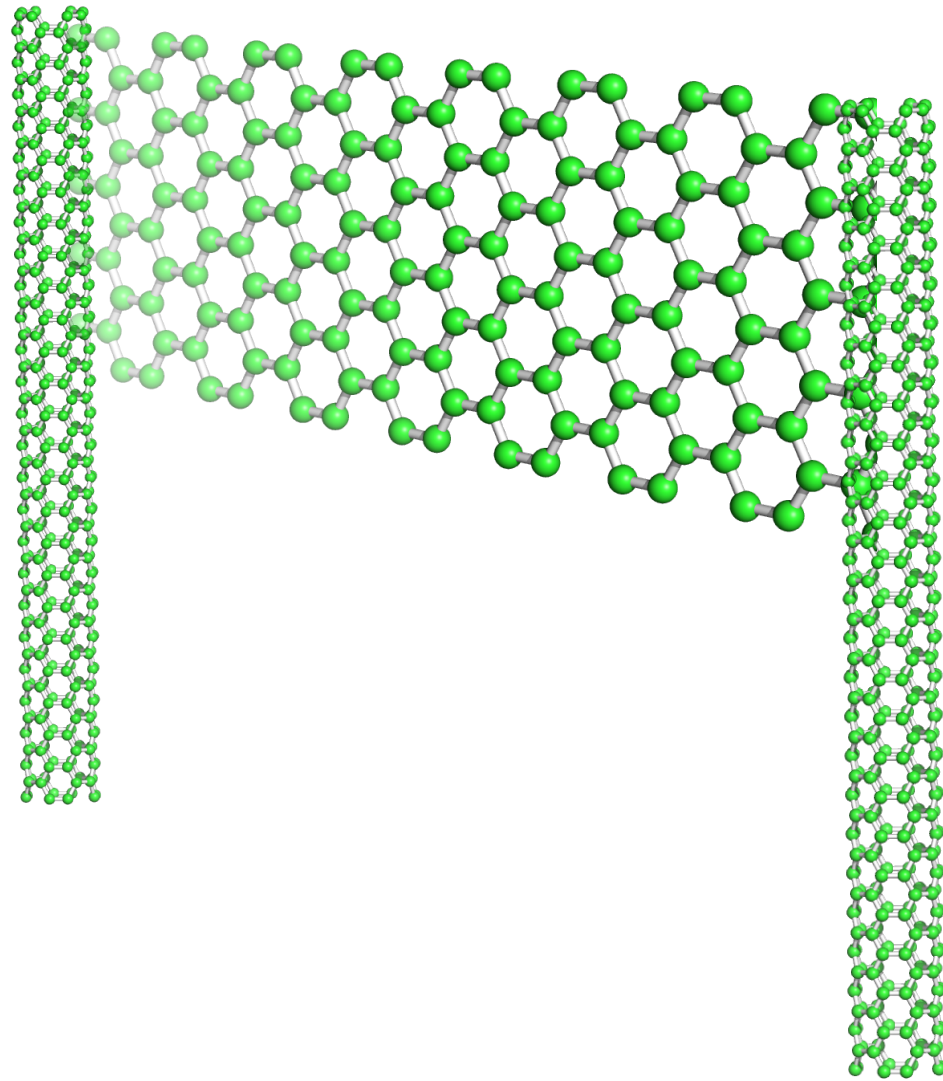
# Fun with Carbon Nanostructures



# Fun with Carbon Nanostructures



# Fun with Carbon Nanostructures



# Crystal Viewer 2.3.4



RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT DONATE TAKE A POLL

## Crystal Viewer Tool

By [Saumitra Raj Mehrotra<sup>1</sup>](#), [Michael Povolotskyi](#), [Sebastian Steiger<sup>1</sup>](#), [Tillmann Christoph Kubis<sup>1</sup>](#), [Abhijeet Paul<sup>1</sup>](#), [Xingshu Sun<sup>1</sup>](#), [Victoria Savikhin<sup>1</sup>](#), [Gerhard Klimeck<sup>1</sup>](#)

1. *Purdue University*

Visualize different crystal lattices and planes


 Edit

Launch Tool

**Archive Version 2.3.4**

Published on 30 Jul 2014 [All versions](#)

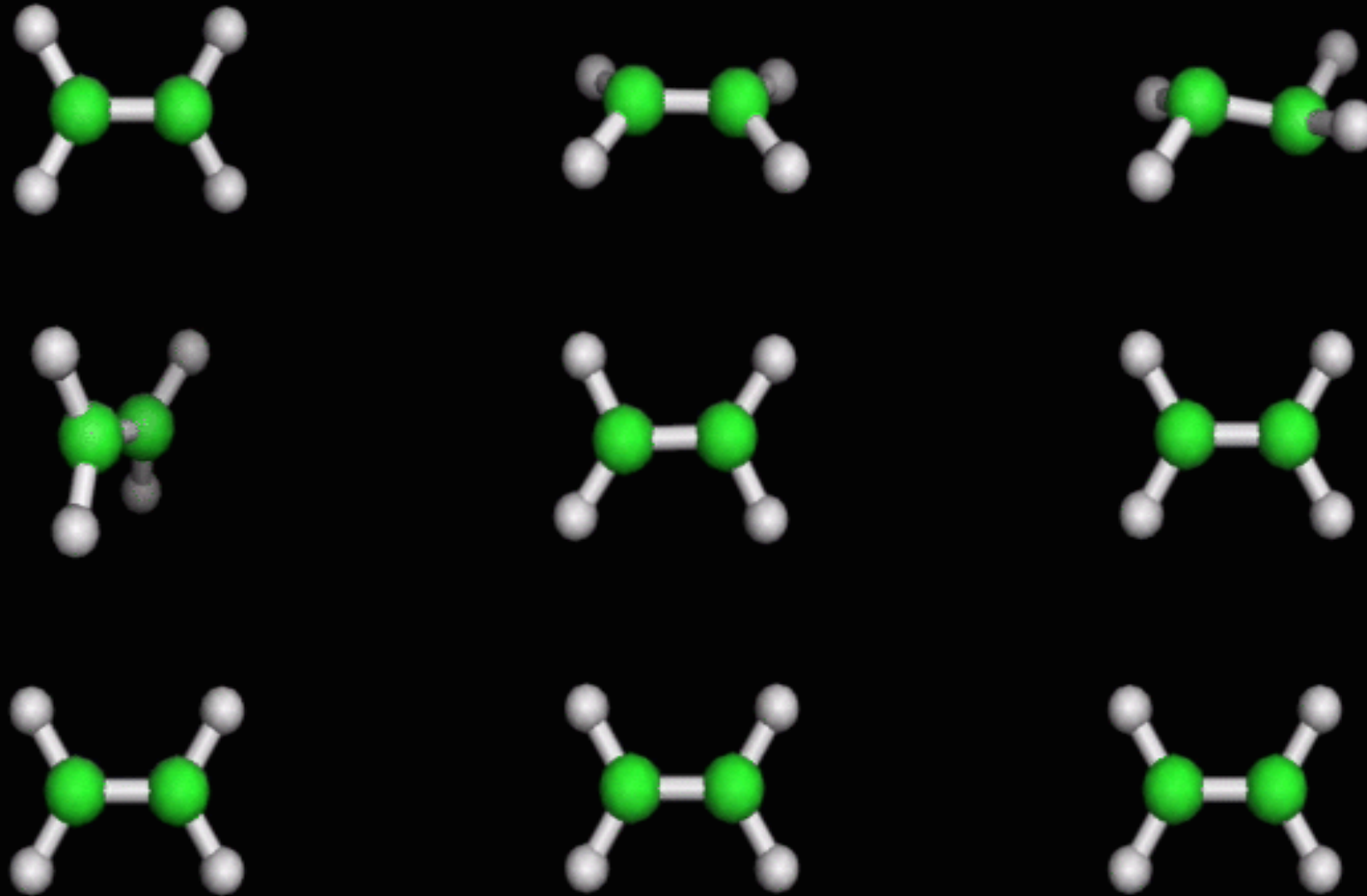
doi:10.4231/D3XK84R2W [cite this](#)

 This tool is closed source.

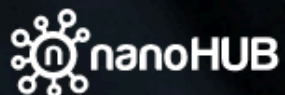
 Newer version available



# Ethene Vibrational Modes



# *ab initio* simulations with ORCA



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Home

## ab initio simulations with ORCA

By [nicolas onofrio](#)<sup>1</sup>, [Alejandro Strachan](#)<sup>1</sup>

1. *Purdue University*

ab initio and density functional theory calculations dedicated to molecular systems

Launch Tool

Version **1.3.3** - published on 22 Jan 2018

doi:10.4231/D32R3P00R [cite this](#)

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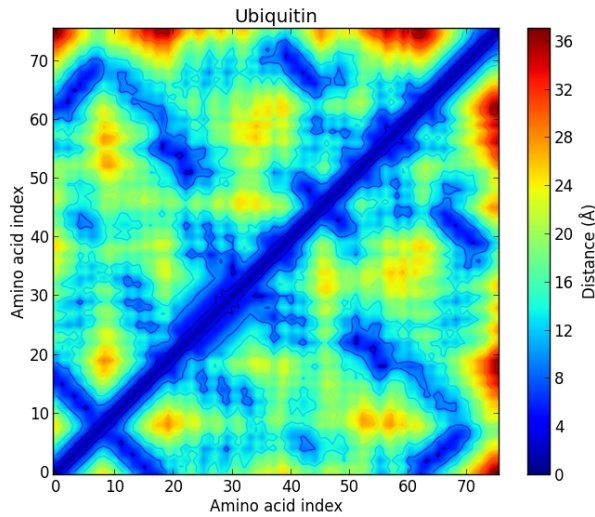


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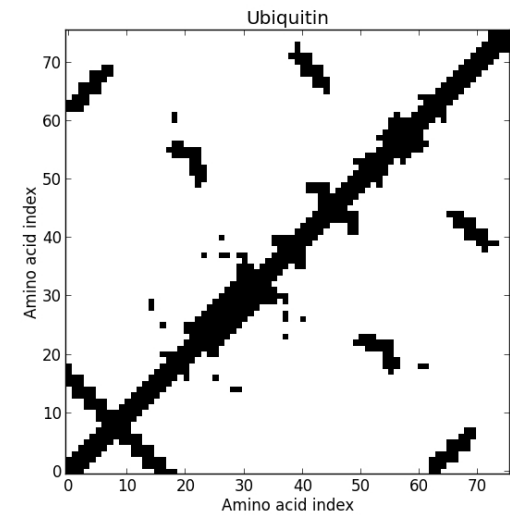
# Ubiquitin (1UBQ)



Molecular  
Structure

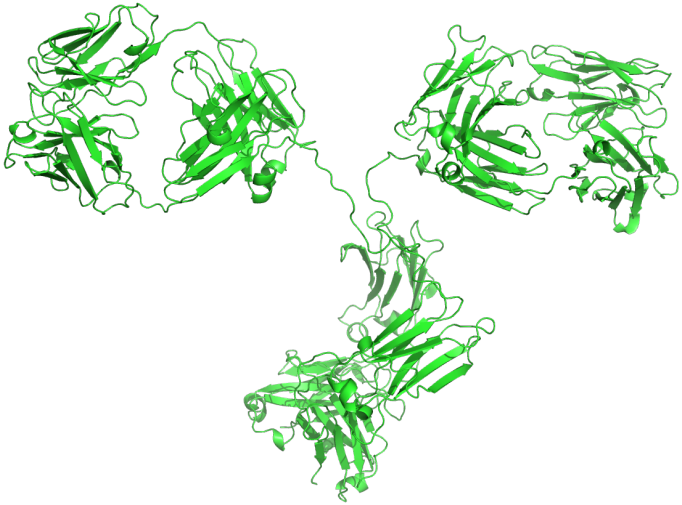


Distance  
Map

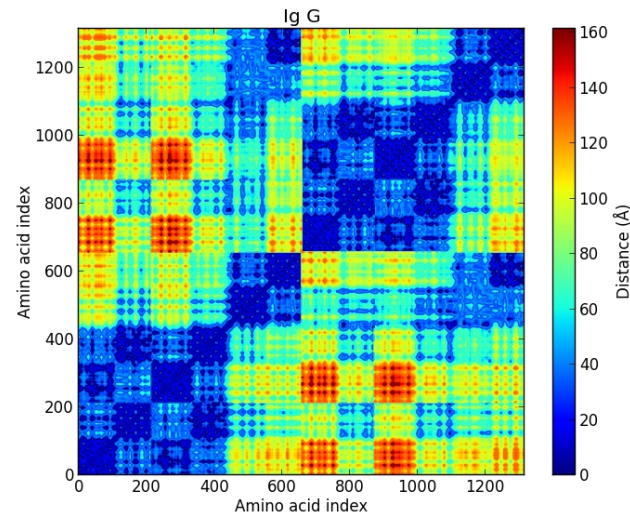


Contact  
Map

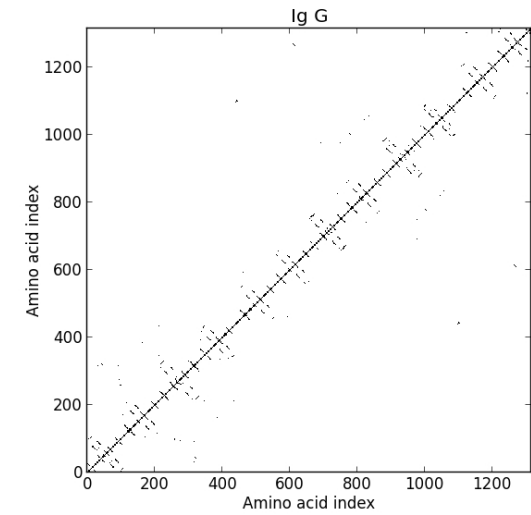
# Immunoglobulin G (1IGT)



Molecular  
Structure



Distance  
Map



Contact  
Map

# Protein Contact Maps



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## Protein Contact Maps

By Benjamin Rafferty<sup>1</sup>, Zachary Carl Flohr<sup>1</sup>, [Ashlie Martini<sup>1</sup>](#)


*1. Purdue University*

Create and view protein contact maps and distance maps.

Launch Tool

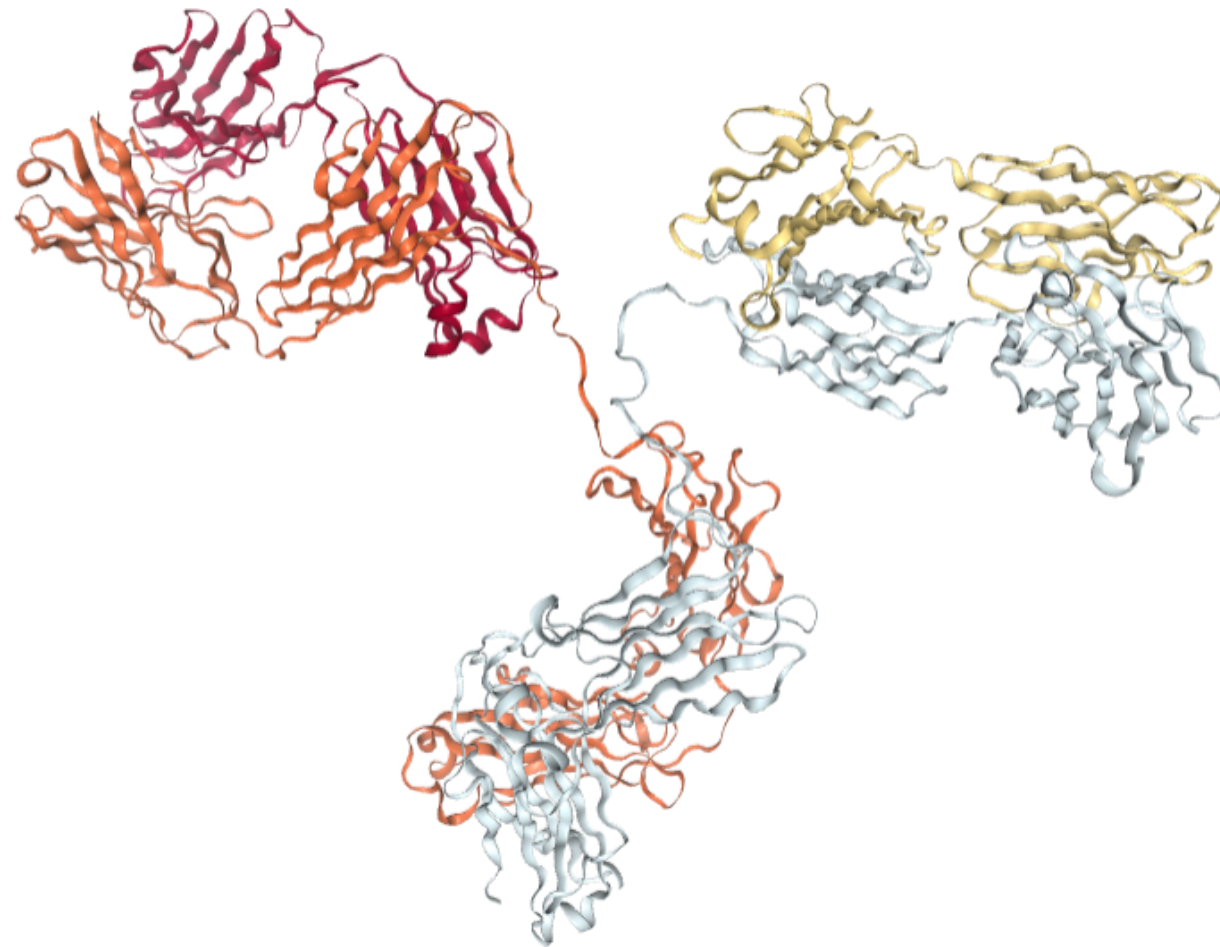
Version **1.3** - published on 25 Aug 2020

doi:10.21981/02DQ-MT84 [cite this](#)

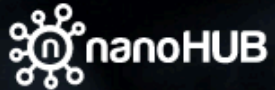
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# Immunoglobulin G (1IGT)



# Demo of Loading and Visualizing Proteins from the RCSB Protein Data Bank



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Home > Tools > Demo of Loading and Visualizing Proteins from the RCSB Protein Data Bank > About

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## Demo of Loading and Visualizing Proteins from the RCSB Protein Data Bank

By [Martin Hunt](#)

Demo of Loading and Visualizing Proteins from the RCSB Protein Data Bank

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Version 1.5 - published on 11 Sep 2018

doi:10.4231/D37659H92 [cite this](#)

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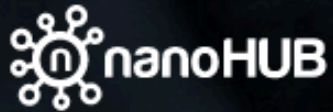
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# Jupyter notebooks in nanoHUB



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Home › Tools


## Jupyter Notebook

Starts the Jupyter notebook server using the latest installed release of anaconda.

Launch Tool

Version **1.7** - published on 27 Jan 2020

doi:10.21981/W6TE-1750 [cite this](#)

 This tool is closed source.



[View All Supporting Documents](#)



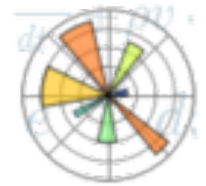
# Jupyter Kernels, Libraries, & Packages in nanoHUB include...



pymatgen



mendeleeev



# nanoHUB Provides Connections to Data



# Managing your Jupyter notebooks

See the handout:

[Setting up Your nanoHUB File Structure in Jupyter Notebooks](#)



# biopython Tutorial

## 2.2 Working with sequences

Disputably (of course!), the central object in bioinformatics is the sequence. Thus, we'll start with a quick introduction to the Biopython mechanisms for dealing with sequences, the `seq` object, which we'll discuss in more detail in [Chapter 3](#).

Most of the time when we think about sequences we have in my mind a string of letters like 'AGTACTGGT'. You can create such `seq` object with this sequence as follows - the ">>>" represents the Python prompt followed by what you would type in:

```
>>> from Bio.Seq import Seq
>>> my_seq = Seq("AGTACTGGT")
>>> my_seq
Seq('AGTACTGGT')
>>> print(my_seq)
AGTACTGGT
```

The `seq` object differs from the Python string in the methods it supports. You can't do this with a plain string:

```
>>> my_seq
Seq('AGTACTGGT')
>>> my_seq.complement()
Seq('TCATGTGACCA')
>>> my_seq.reverse_complement()
Seq('ACCAGTGTACT')
```

**mendeleev****Contents**[Quick overview](#)[Installation](#)[Tutorials](#)[mendeleev tutorial](#)[Accessing the data in bulk](#)[Plotting tutorial](#)[Visualizing properties](#)[Custom properties](#)[Wide 32-column version](#)[Jupyter notebooks](#)[Data](#)[Electronegativities](#)[API Reference](#)[License](#)[Changes](#)


## Plotting tutorial

The plotting module is based on the [Bokeh](#) package and enables visualization of various properties of elements. The plotting in the form of periodic table is done by the `periodic_plot` function that takes a [pandas](#) `DataFrame`.

To embed the plots in the [jupyter notebook](#) first the `BokehJS` needs to be started.

```
[1]: from bokeh.plotting import output_notebook, output_file
```

```
[2]: output_notebook()
```

 BokehJS 2.0.1 successfully loaded.

Now we can get the data from `mendeleev` as a `pandas DataFrame` through `get_table` method

```
[3]: from mendeleev import get_table
      from mendeleev.plotting import periodic_plot
```

```
[4]: ptable = get_table('elements')
```

To plot the default table pass the `ptable` to the `periodic_plot` function

```
[5]: periodic_plot(ptable)
```

# Machine Learning for Materials Science

Collect

## Machine Learning for Materials Science: Part 1

By [Juan Carlos Verduzco Gastelum<sup>1</sup>](#), [Alejandro Strachan<sup>1</sup>](#), [Saaketh Desai<sup>1</sup>](#)


1. [Purdue University](#)

Machine learning and data science tools applied to materials science

Launch Tool

Version 1.3 - published on 01 Apr 2020

doi:10.21981/WGQC-3249 [cite this](#)

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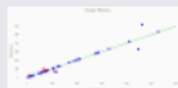
Questions

Reviews

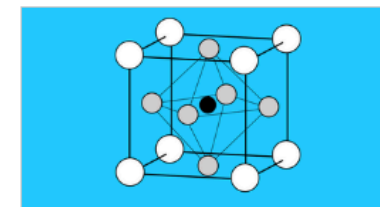
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01 Apr 2020



# Introduction to Machine Learning for Materials Science

The tutorials here will give you an insight into the usage of Machine Learning to approach problems related to materials science.

- **Get started** Click on the links below to begin each tutorial.
- **Important** To exit individual tutorials and return to this page, use File -> Close and Halt. "Terminate Session" (top right) will kill your entire Jupyter session.

## [Querying databases, Organizing and Plotting Data:](#)

- Query Pymatgen and Mendeleev for properties like Young's modulus and melting temperature
- Organize data into Pandas dataframes and python dictionaries and plot using Plotly

## [Linear Regression to predict material properties:](#)

- Perform linear regression using the scikit learn package and predict Young's modulus
- Visualize trends in data and 'goodness of fit' of linear model

## [Neural Network Regression to predict material properties:](#)

- Use neural networks to perform non-linear, higher order regression
- Visualize trends and compare non-linear model to linear regression

## [Neural Network Classification to predict crystal structures:](#)

- Use neural networks to classify elements according to their crystal structures

# Hands-on Data Science and Machine Learning Training

By [Alejandro Strachan](#)<sup>1</sup>, [Saaketh Desai](#)<sup>2</sup>

1. *Materials Engineering, Purdue University, West Lafayette, IN* 2. *Purdue University, West Lafayette, IN*

<https://nanohub.org/resources/33245>

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[Slides/Notes podcast](#)

- Introduction to Jupyter Notebooks, Data Organization and Plotting
- Repositories and Data Management
- Hands-on Supervised Learning: Part 1 - Linear Regression and Neural Networks
- Hands-on Supervised Learning: Part 2 - Classification and Random Forests
- Hands-on Sequential Learning and Design of Experiments



Saaketh Desai



Zachary McClure



Michael Sakano

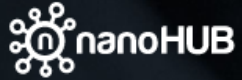


Juan Carlos Verduzco

A course that  
uses Jupyter  
notebook tools



# Video tutorials to accompany the mseml notebooks



## Hands-on Data Science and Machine Learning Training

By [Alejandro Strachan](#)<sup>1</sup>, [Saaketh Desai](#)<sup>2</sup>

1. *Materials Engineering, Purdue University, West Lafayette, IN* 2. *Purdue University, West Lafayette, IN*

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