

**1.021, 3.021, 10.333, 22.00** Introduction to Modeling and Simulation  
Spring 2018

# Recitation #1

nanoHUB and Visual Molecular Dynamics

- **Recitation instructor:** Francisco Martin-Martinez

email: [fmartinm@mit.edu](mailto:fmartinm@mit.edu)



**Massachusetts Institute of Technology**

**Recitation instructor:**

Francisco Martin-Martinez (office 1-235, [fmartimm@mit.edu](mailto:fmartimm@mit.edu))  
*Department of Civil and Environmental Engineering*

**Office hours:** TBA

**Recitations:**

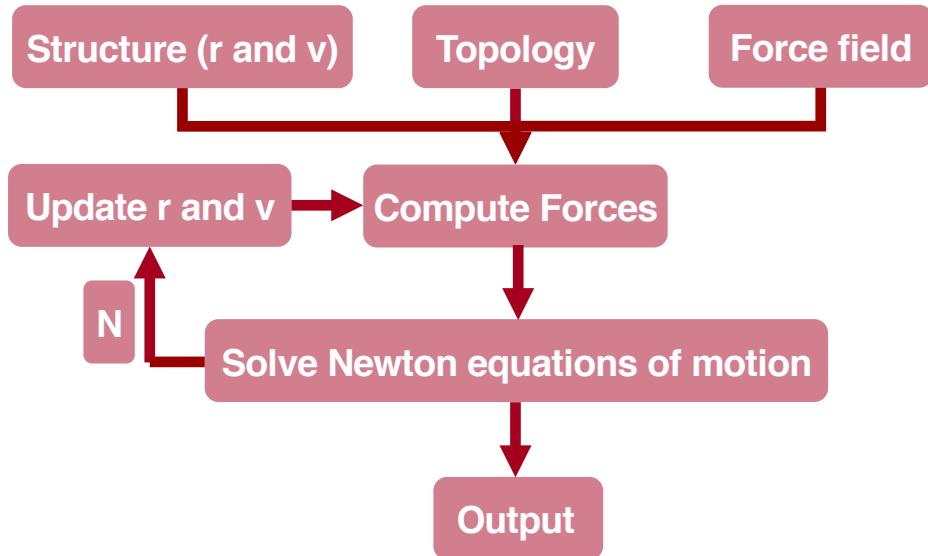
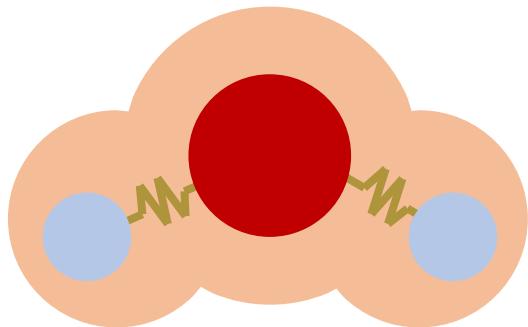
Monday and Friday 4-5 pm in 8-205  
“Identical” versions of recitations given

**Let’s do groups!**

# Summary on molecular dynamics

Atoms considered as spheres connected by springs

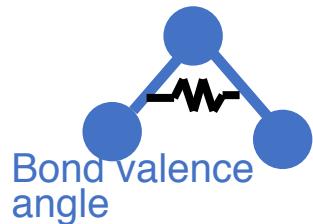
## Force field



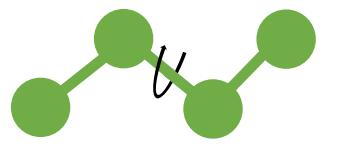
$$V(r) = \sum_{Bonds} K_b(b - b_0)^2 + \sum_{Angles} K_\theta(\theta - \theta_0)^2 + \sum_{Dihedrals} K_\chi(1 + \cos(n_\chi - \delta)) + \sum_{Non-bonded} \left[ \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} - \epsilon_{ij} \left\{ \left( \frac{R_{min,ij}}{r_{ij}} \right)^{12} - 2 \left( \frac{R_{min,ij}}{r_{ij}} \right)^6 \right\} \right]$$



Bond length



Bond valence angle



Bond dihedral angle

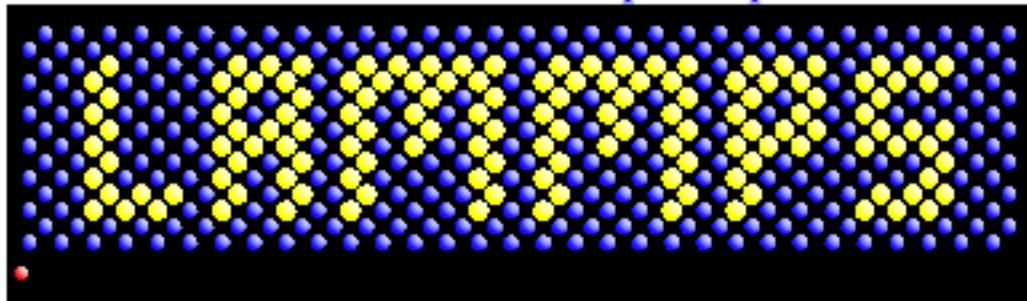


Electrostatic



van der Walls

# Molecular dynamics codes



<http://lammps.sandia.gov>

Example: protein folding

<https://www.youtube.com/watch?v=gFcp2Xpd29I>

Advice: Learn Linux/Unix

# Our too: nanoHUB – nanohub.org



RESOURCES EXPLORE NANOHUB-U PARTNERS COMMUNITY ABOUT SUPPORT

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# NANO is HUGE

LARGEST NANOTECHNOLOGY ONLINE RESOURCE

400  
simulation tools

1.4M  
users

4500  
resources

# Our too: nanoHUB – nanohub.org

A web-based resource containing diverse simulations tools for:

- Nanoscience, nanotechnology and related fields

**More than 330 well-maintained tools**

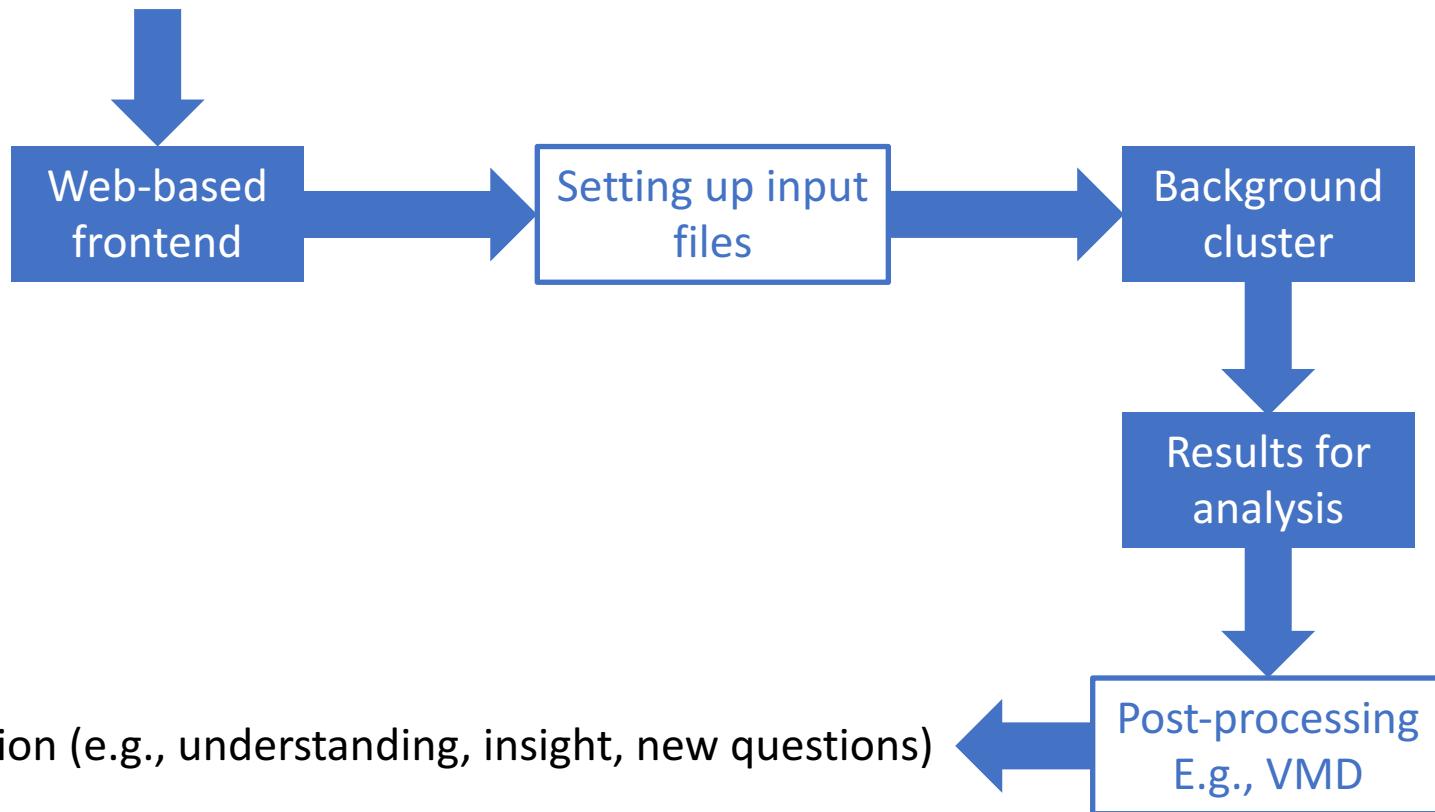
You can:

- Simulate various nanoscopic phenomena
- Do your own research
- Learn nanoscience
- Develop your own tools

Use free of charge (funded by NSF)

# nanoHUB Workflow

Physical problem (e.g., deformation, electronic properties, fracture, diffusion)



nanoHUB

# Our too: nanoHUB – nanohub.org



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Create new account

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With an affiliated institution:

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Sign in with LinkedIn

**i** You can choose to log in via one of these services, and we'll help you fill in the info below!

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## Duo Authentication

Duo second-factor authentication is required.

Choose an authentication method



Duo Push Send me a Push

Call Me Call Me

Enter a Passcode Enter a Passcode

Remember me for 30 days

[What is this? !\[\]\(aca27db703fc917451dfe701336453db\_img.jpg\)](#) [Need help?](#)

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Follow the steps and fill  
in your profile

## Old sessions, reopen/kill

MY SESSIONS

No active sessions found.

Storage (manage)

5% of 10GB

## Tools you have used

MY TOOLS

Recent Favorites All Tools

Polymer Modeler

Atomic Stick-Slip

Nanowire Tensile Deformation Lab

REBO

RESOURCES

- Learning Modules
- Teaching Materials
- Online Seminars
- Animations
- Workshops
- Downloads

New tab

POLLS

How would you describe your use of nanoHUB.org?

I use nanoHUB.org on a regular basis

I have used nanoHUB.org at times for specific purposes and expect to use it again

I have used nanoHUB.org at times for specific purposes and

WHAT'S NEW MY INTERESTS

[Add Interests] My Interests:

There are no new items.

More new resources >

# Visual Molecular Dynamics (VMD)

*Download standalone  
program to your own computer*

# <http://www.ks.uiuc.edu/Research/vmd/>

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Type Keywords  SEARCH

THEORETICAL and COMPUTATIONAL BIOPHYSICS GROUP



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VMD Visual Molecular Dynamics

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS X, Unix, or Windows, is distributed free of charge, and includes source code.  
[\(more details...\)](#)

**Spotlight**

VMD is frequently used to make figures and illustrations that grace the cover pages of textbooks and journals. A sampling of some of the VMD cover page images produced by local researchers and collaborators can be viewed [here](#).

**Other Spotlights**

**Structure**



**Overview**

Molecular representations  
VMD plugin library  
Molecular file formats  
GPU-accelerated computing  
Interactive molecular dynamics  
Programs that use VMD  
VMD research publications  
How to cite VMD  
VMD citation list (19,000 as of Oct'16)

**Download** 

Download  
Download (all versions)  
VMD 1.9.3 (MacOS X, Unix, Windows)  
VMD 1.9.2 (MacOS X, Unix, Windows)  
VMD 1.9.1 (MacOS X, Unix, Windows)  
VMD script library  
License, Copyright and Disclaimer

**VMD Mailing List**

**VMD Tutorials**

**VMD Manuals**

**VMD Community Pages**

**News and Announcements**

J. Physical Chemistry B, Klaus Schulten Memorial Issue, 2017 NEW  
Challenges of Integrating Stochastic Dynamics and Cryo-electron Tomograms in Whole-cell Simulations, JPCB 2017 NEW  
VMD 1.9.3 (MacOS X, Unix, Windows)  
GPU-Accelerated Molecular Dynamics Clustering Analysis with OpenACC, Parallel Programming with OpenACC, 2016  
Early Experiences Porting the NAMD and VMD Molecular Simulation and Analysis Software to GPU-Accelerated OpenPOWER Platforms, LNCS 2016  
Immersive Molecular Visualization with Omnidirectional Stereoscopic Ray Tracing and Remote Rendering, HPDAV 2016  
High Performance Molecular Visualization: In-Situ and Parallel Rendering with EGL, HPDAV 2016  
Evaluation of Emerging Energy-Efficient Heterogeneous Computing Platforms for Biomolecular and Cellular Simulation Workloads, HCW 2016  
Molecular dynamics-based refinement and validation for sub-5Å cryo-electron microscopy maps, eLife 2016  
QwikMD - Integrative Molecular Dynamics Toolkit for Novices and Experts, Scientific Reports 2016  
TopoGromacs: Automated Topology Conversion from CHARMM to GROMACS within VMD, JCIM 2016  
Atomic Detail Visualization of Photosynthetic Membranes with GPU-Accelerated Ray Tracing, J. Par. Comp. 2016  
Past announcements

**Gallery**

Chromatophore VR demo (VMD + Unreal Game Engine) shown in NVIDIA booth at SC'16  
Example VMD VR/3-D YouTube videos  
Chemical Visualization of Human Pathogens: the Retroviral Capsids, Finalist, SC'15 Viz. Showcase  
Visualization of Energy Conversion Processes in a Light Harvesting Organelle at Atomic Detail, 1st Place Winner, SC'14 Viz. Showcase  
VMD movie gallery on YouTube

## Software Downloads

### Download VMD:

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. Visit the [VMD website](#)

Selecting an archive below will lead to a user registration and login page. Your download will continue after you have registered or logged in.

#### Version 1.9.4 LATEST ALPHA (2017-12-21) Platforms:

Latest pre-release ALPHA test version

- [LINUX\\_64 OpenGL, CUDA, OptiX, OSPRay](#) (Linux (RHEL 6.7 and later) 64-bit Intel/AMD x86\_64 SSE, with CUDA 9.x, OptiX, OSPRay)
- [MacOS X OpenGL \(32-bit Intel x86\)](#) (Apple MacOS-X (10.10.x or later) with hardware OpenGL (native bundle))

#### Version 1.9.3 (2016-11-30) Platforms:

We recommend that all users upgrade to VMD 1.9.3

- [Source Code](#)
- [LINUX\\_64 OpenGL, CUDA, OptiX, OSPRay](#) (Linux (RHEL 6.7 and later) 64-bit Intel/AMD x86\_64 SSE, with CUDA 8.x, OptiX, OSPRay)
- [LINUX\\_64 Text-mode w/ EGL](#) (Linux (RHEL 6.7 and later) 64-bit Intel/AMD x86\_64 w/ SSE, Text-mode w/ EGL)
- [LINUX\\_64 Text-mode](#) (Linux (RHEL 6.7 and later) 64-bit Intel/AMD x86\_64 w/ SSE, Text-mode)
- [LINUX MIC-AVX512 Text-mode](#) (Linux (RHEL 6.7 and later) 64-bit Intel Xeon Phi MIC w/ AVX-512, Text-mode, OSPRay)
- [LINUX MIC-AVX512, OpenGL, CUDA, OptiX, OSPRay](#) (Linux (RHEL 6.7 and later) 64-bit Intel Xeon Phi MIC w/ AVX-512, OpenGL, CUDA7.5, OptiX, OSPRay)
- [LINUX OpenPOWER Text-mode](#) (Linux 64-bit IBM OpenPOWER w/ VSX, Text-mode)
- [MacOS X OpenGL \(32-bit Intel x86\)](#) (Apple MacOS-X (10.4.7 or later) with hardware OpenGL (native bundle))
- [Windows OpenGL, CUDA](#) (Windows XP/Vista/7/8/10 (32-bit) with OpenGL and CUDA)
- [Windows OpenGL](#) (Microsoft Windows XP/Vista/7/8/10 (32-bit) using OpenGL)
- [NCSA Blue Waters \(Cray XK7 w/ OpenGL\)](#) (NCSA Blue Waters (Cray XK7) MPI, CUDA, OpenGL Pbuffers, TachyonL-OptiX)
- [ORNL Titan \(Cray XK7\)](#) (ORNL Titan (Cray XK7) MPI, CUDA, TachyonL-OptiX)
- [CSCS Piz Daint \(Cray XC50 w/ EGL\)](#) (CSCS Piz Daint (Cray XC50) MPI, CUDA, EGL Pbuffers, TachyonL-OptiX)

**First and Last Name:**

**Email Address:**

**Affiliation:**

- Academic  Government  Industrial  Other (specify)

**The number of people using TCBG software at my site is:**

- 1  2-4  5-10  11-20  21 or more

**I use TCBG software primarily for:**

- Research  Teaching  Commerce  Personal

**The work I do with TCBG software is funded (at least partially) by NIH:**

- Yes  No

**Re-enter password for confirmation:**

**Register**

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VMD script library  
License, Copyright and Disclaimer

**VMD Manuals** ←

**Documentation and Support**

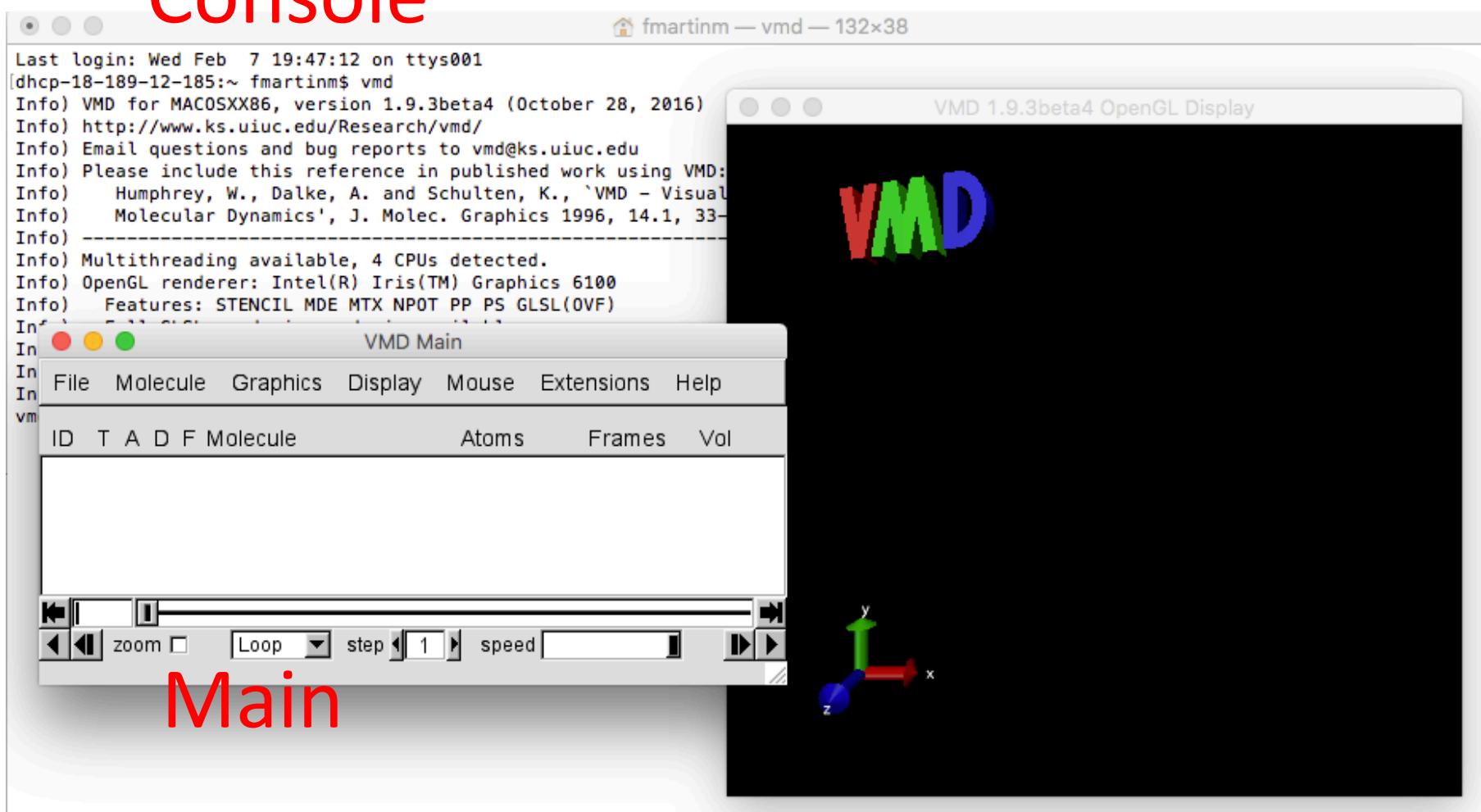
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# Console



Open GL

# Protein Data Bank: 130K+ protein structures

<http://www.rcsb.org>

The screenshot shows the RCSB PDB homepage. On the left, a sidebar menu includes: Welcome, Deposit, Search, Visualize, Analyze, Download, and Learn. The main content area features a large search bar at the top right. Below it, a section titled "A Structural View of Biology" discusses the archive's role in understanding 3D shapes of biomolecules. A video thumbnail for "WHAT IS A PROTEIN?" is shown. To the right, a "February Molecule of the Month" section displays two molecular models of EPSP Synthase and Weedkillers.

RCSB PDB PROTEIN DATA BANK

137478 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

Search by PDB ID, author, macromolecule, sequence, or ligands

Advanced Search | Browse by Annotations

PDB-101 Worldwide PDB EMDDataBank NDB Worldwide Protein Data Bank Foundation

Go

f t y

## A Structural View of Biology

This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

As a member of the wwPDB, the RCSB PDB curates and annotates PDB data. The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

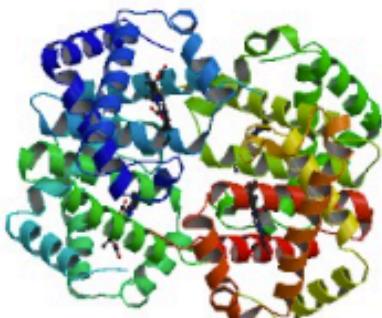
### New Video: What is a Protein?

VIDEO WHAT IS A PROTEIN?

## February Molecule of the Month

EPSP Synthase and Weedkillers

# Search for a protein e.g., Hemoglobin



 3D View

1A3N

DEOXY HUMAN HEMOGLOBIN

[Tame, J.R.](#), [Vallone, B.](#)

(2000) Acta Crystallogr D Biol Crystallogr **56** 805-811

**Released:** 4/29/1998

**Method:** X-ray Diffraction

**Resolution:** 1.8 Å

**Residue Count:** 574

CIF 

[Download File](#)

[View File](#)



Crystallographic information file

**Macromolecule:**

HEMOGLOBIN (ALPHA CHAIN) (protein)

HEMOGLOBIN (BETA CHAIN) (protein)

**Unique Ligands:** [HEM](#)

**Search term match score:** 260.80

**Matched fields in 1A3N.cif:**

- **\_entity.pdbx\_description:** HEMOGLOBIN (ALPHA CHAIN), HEMOGLOBIN (BETA CHAIN), PROTOPORPHYRIN IX CONTAINING FE
- **\_struct.title:** DEOXY HUMAN HEMOGLOBIN



Structure Summary    3D View    Annotations    **Sequence**    Sequence Similarity    Structure Similarity    Experiment

Display Files ▾    Download Files ▾

Biological Assembly 1

**1A3N**

DEOXY HUMAN HEMOGLOBIN

DOI: [10.2210/pdb1A3N/pdb](https://doi.org/10.2210/pdb1A3N/pdb)

Classification: [OXYGEN TRANSPORT](#)

Organism(s): [Homo sapiens](#)

Deposited: 1998-01-22 Released: 1998-04-29

Deposition Author(s): [Tame, J.](#), [Vallone, B.](#)

Experimental Data Snapshot

Method: X-RAY DIFFRACTION  
Resolution: 1.8 Å  
R-Value Free: 0.220  
R-Value Work: 0.171

wwPDB Validation

3D Report Full Report

Metric	Percentile Ranks	Value
Rfree	2	0.207
Clashscore	0	2
Ramachandran outliers	0	2.2%
Sidechain outliers	2.2%	0.5%
RSRZ outliers	0	0.5%

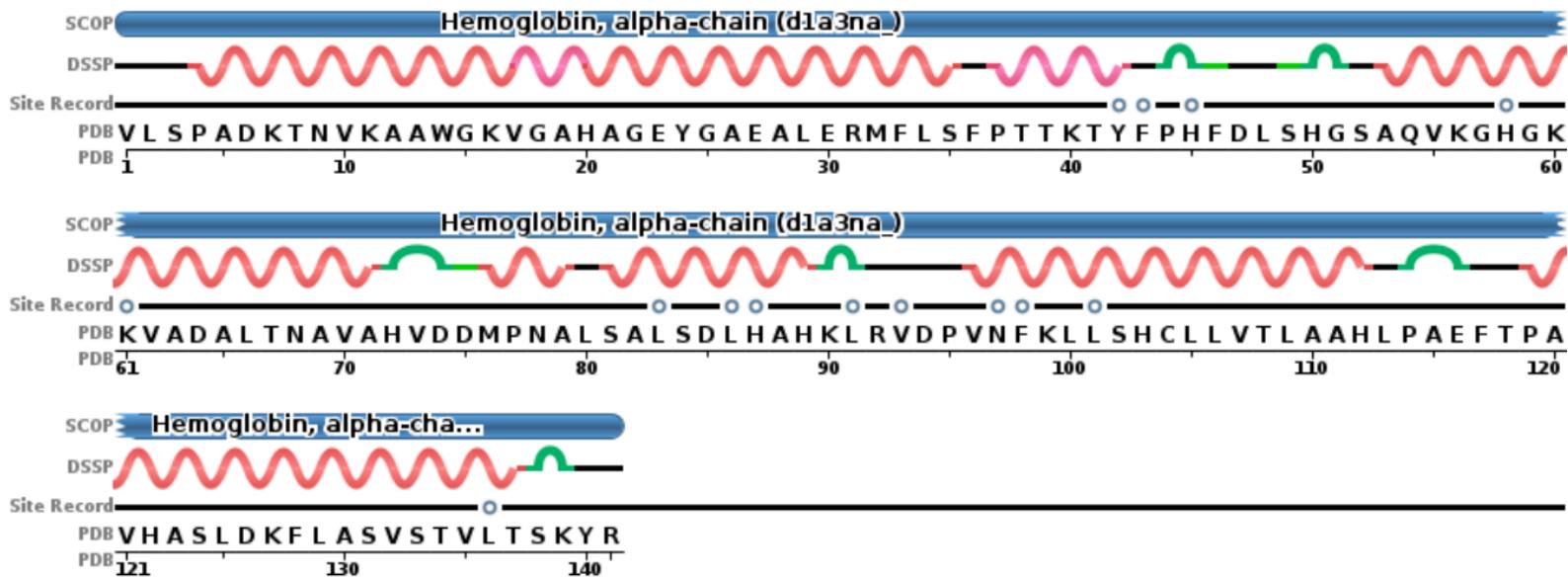
Worse    Better

Percentile relative to all X-ray structures

Percentile relative to X-ray structures of similar resolution

3D View: [Structure](#) | [Electron Density](#) | [Ligand Interaction](#)

## Sequence Chain View



### Site Record Legend

- BINDING SITE FOR RESIDUE HEM A 142 (Software)

### DSSP Legend

— empty: no secondary structure assigned

S: bend



T: turn

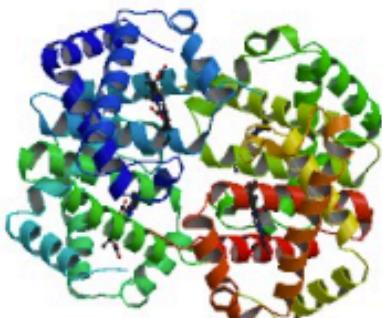


G: 3/10-helix



H: alpha helix

# Search for a protein e.g., Hemoglobin



 3D View

1A3N

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[Tame, J.R.](#), [Vallone, B.](#)

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[Download File](#)

[View File](#)



Crystallographic information file

**Macromolecule:**

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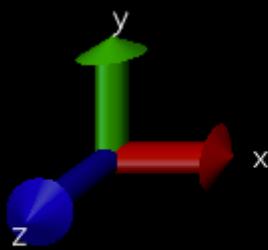
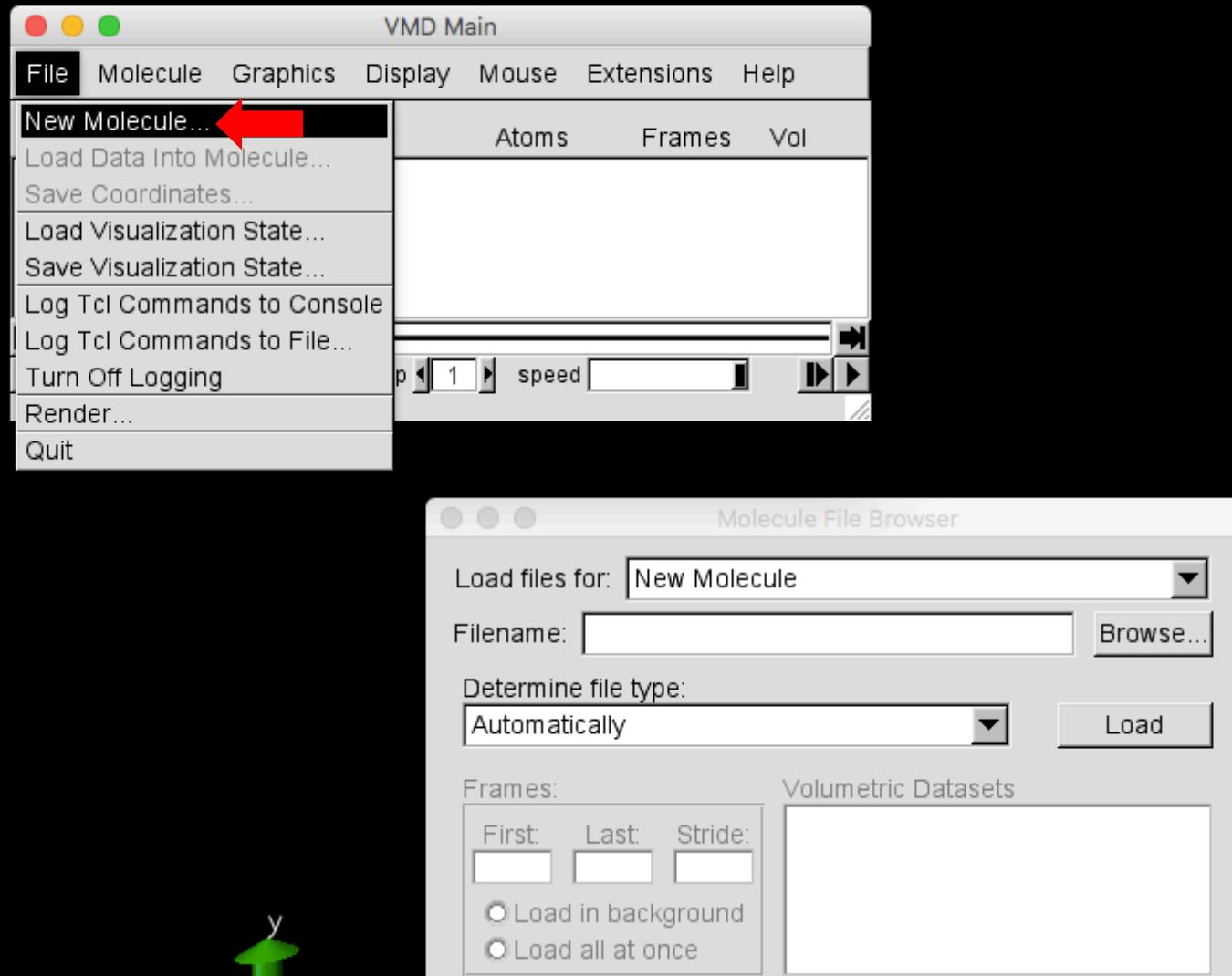
HEMOGLOBIN (BETA CHAIN) (protein)

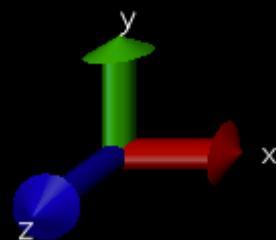
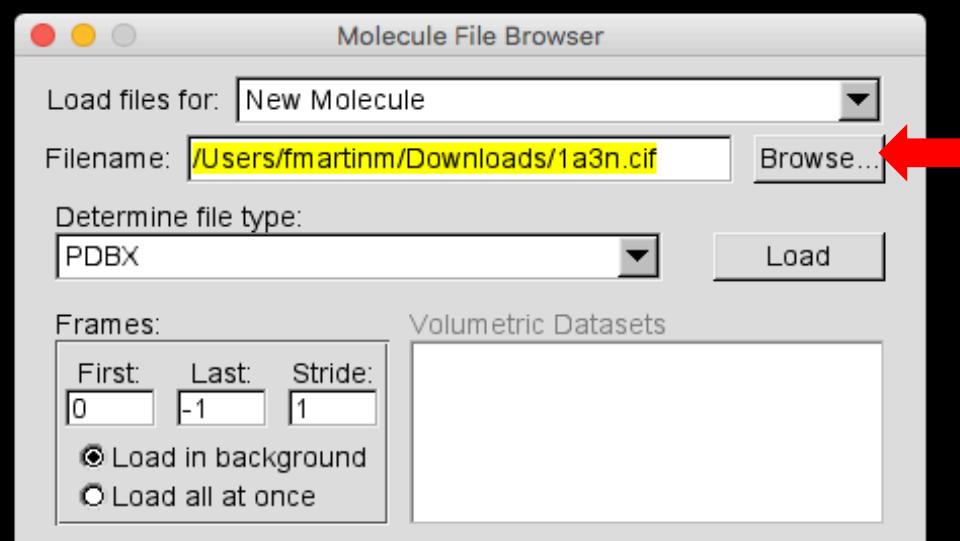
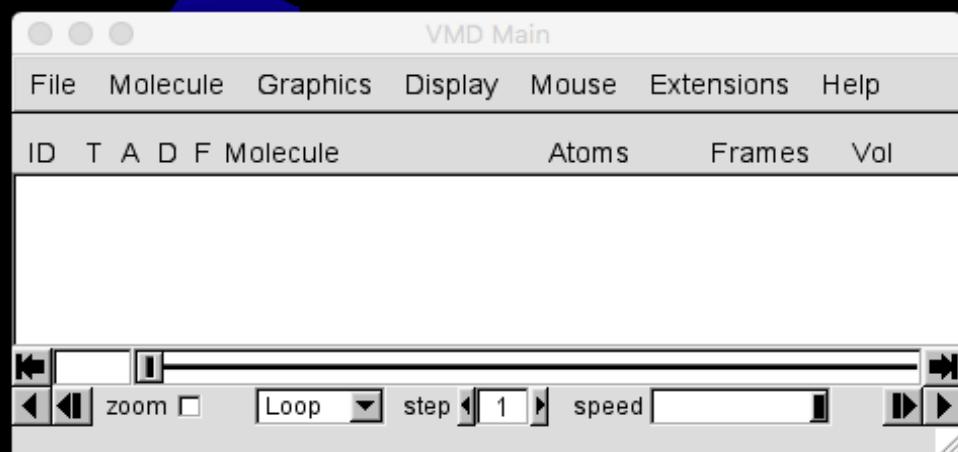
**Unique Ligands:** [HEM](#)

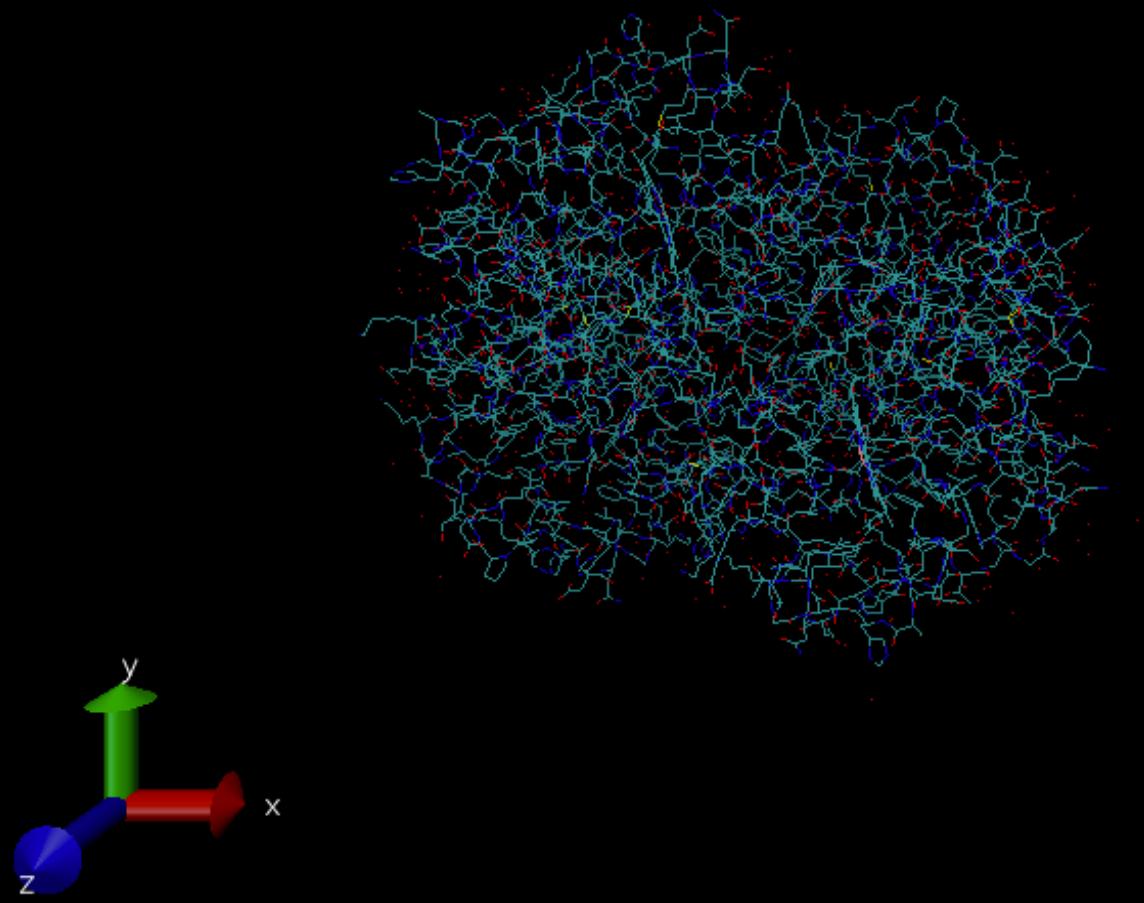
**Search term match score:** 260.80

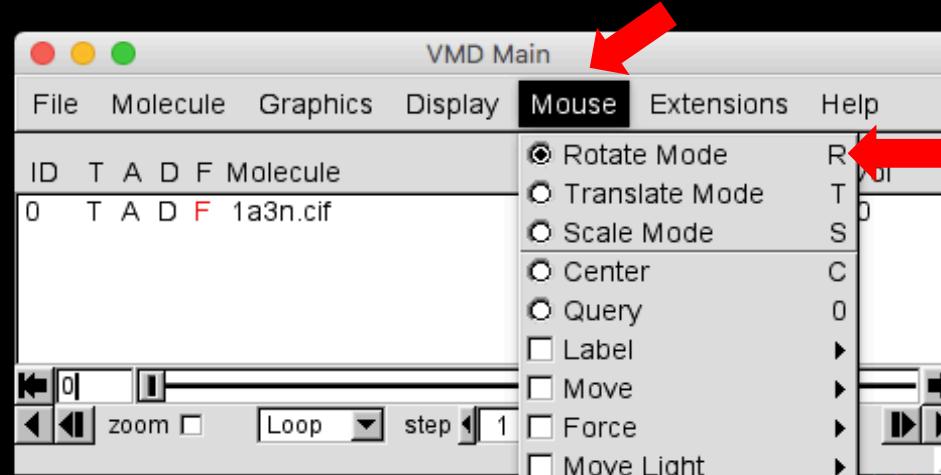
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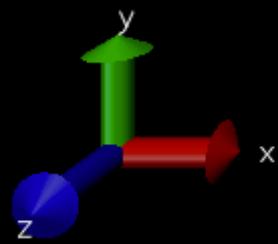
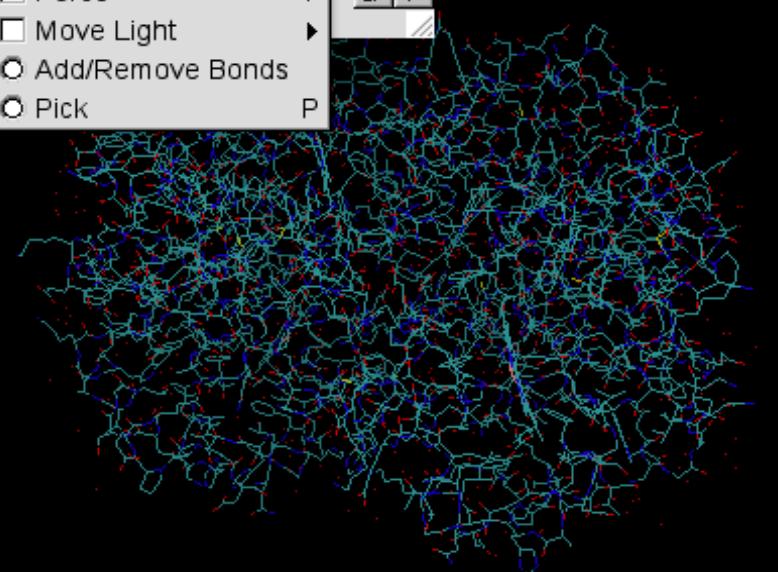


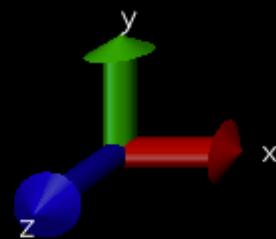
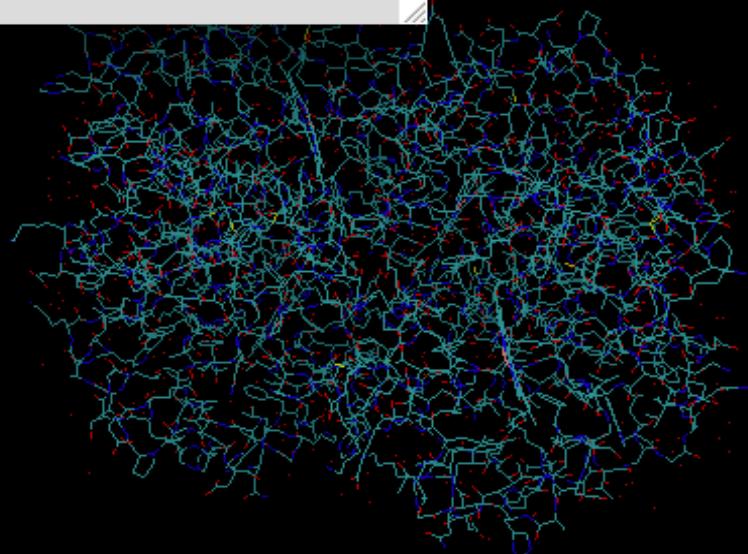
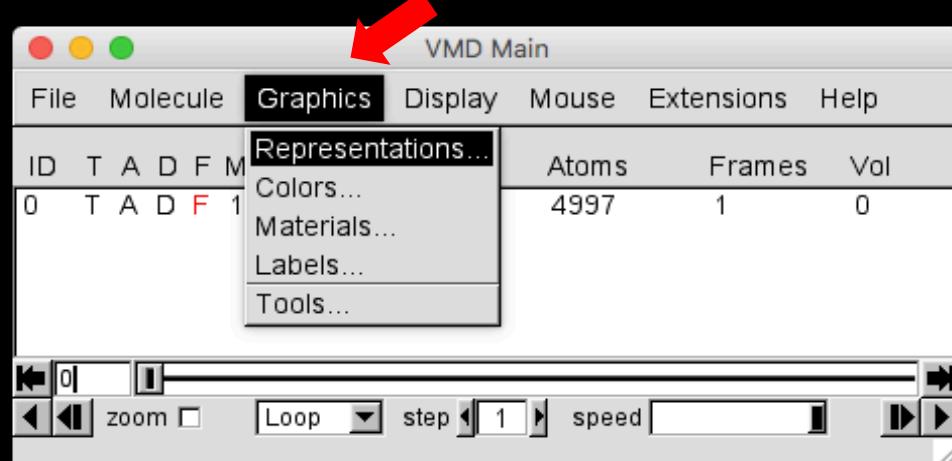


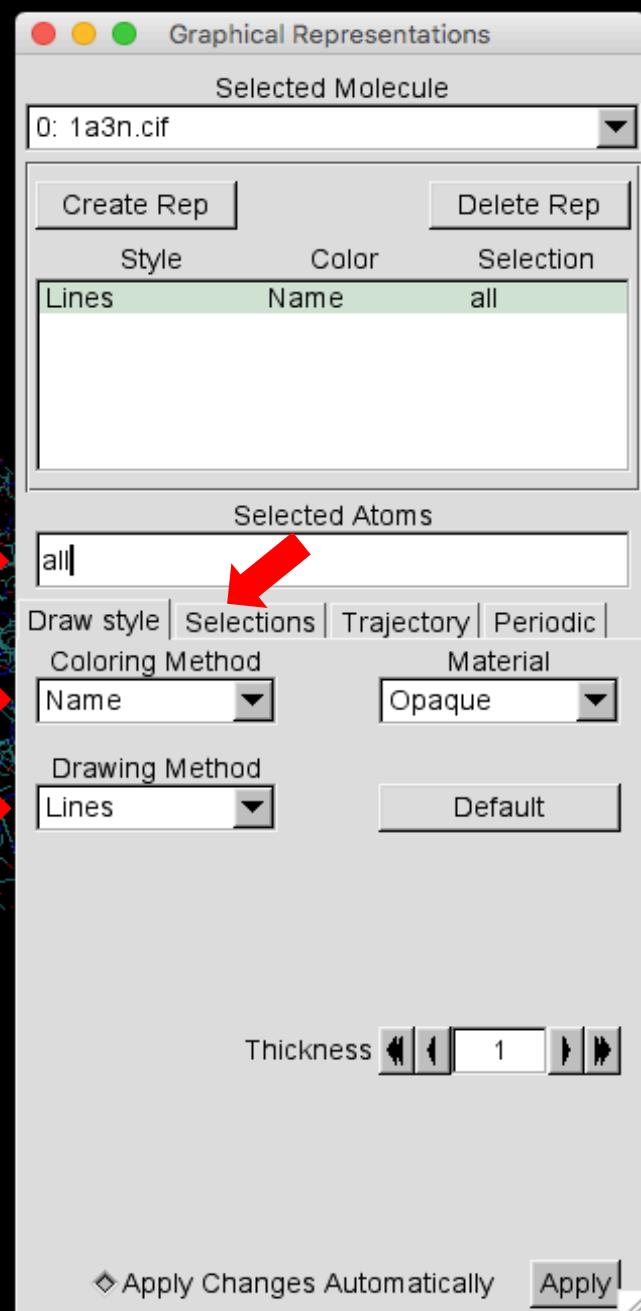
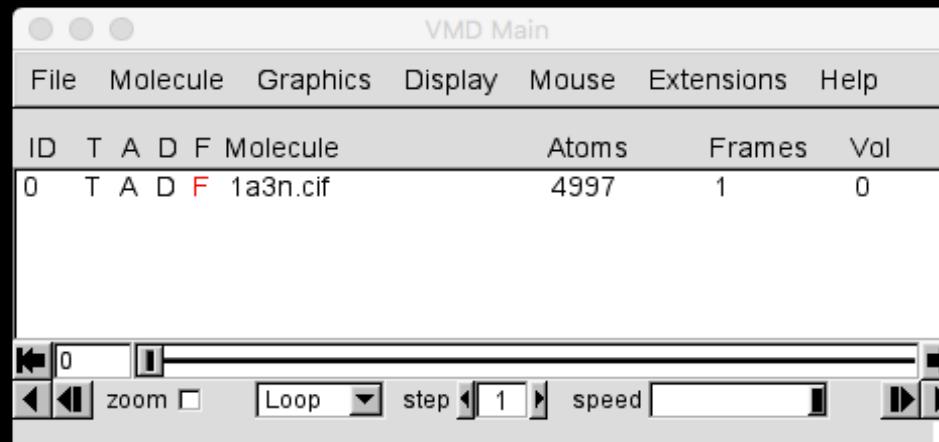




- Rotate Mode R
- Translate Mode T
- Scale Mode S
- Center C
- Query Q
- Label ▶
- Move ▶
- Force ▶
- Move Light ▶
- Add/Remove Bonds P
- Pick





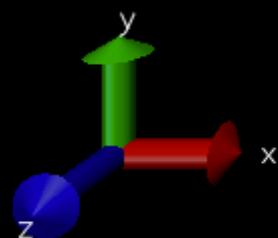
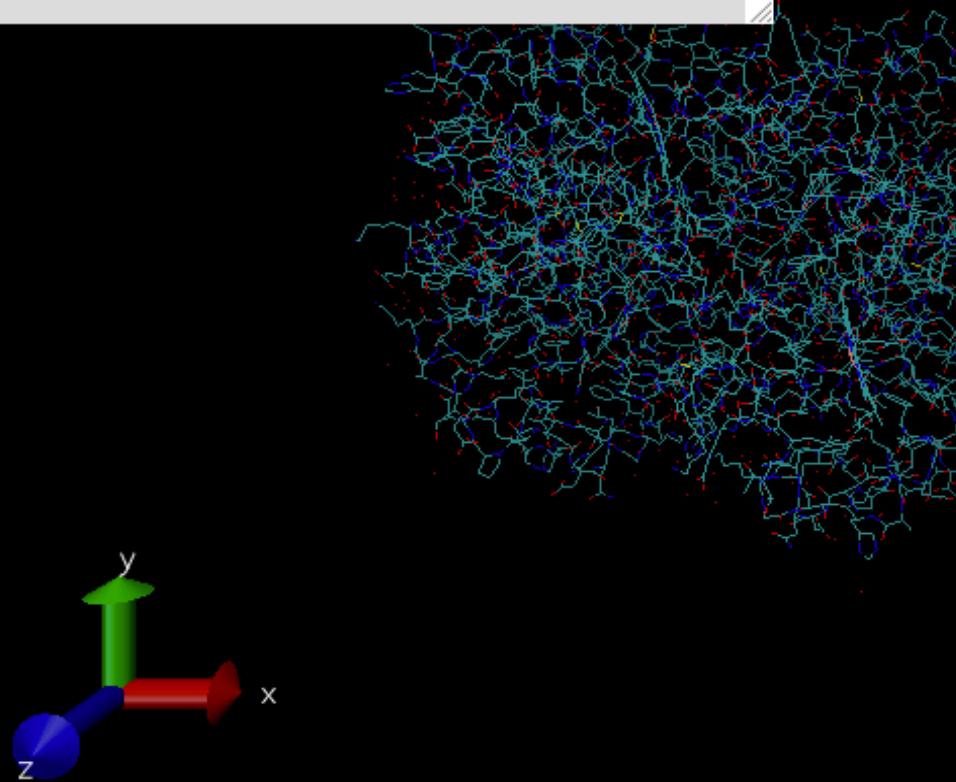


VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	<b>F</b>	1a3n.cif	4997	1	0

← 0 → zoom □ Loop step □ 1 speed □ ▶ ▶



Graphical Representations

Selected Molecule  
0: 1a3n.cif

Create Rep Delete Rep

Style Color Selection

Lines	Name	all
-------	------	-----

Selected Atoms  
all

Draw style | Selections | Trajectory | Periodic |  
Coloring Method Material

Name Opaque

Drawing Method  
Lines Default  
Bonds  
DynamicBonds  
HBonds  
Points  
VDW  
CPK  
Licorice  
Polyhedra  
Trace  
Tube  
**Ribbons**  
NewRibbons  
Cartoon  
NewCartoon

Thickness □ 1 □

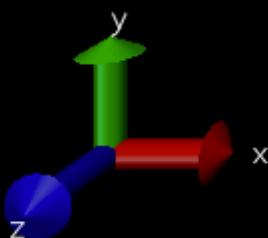
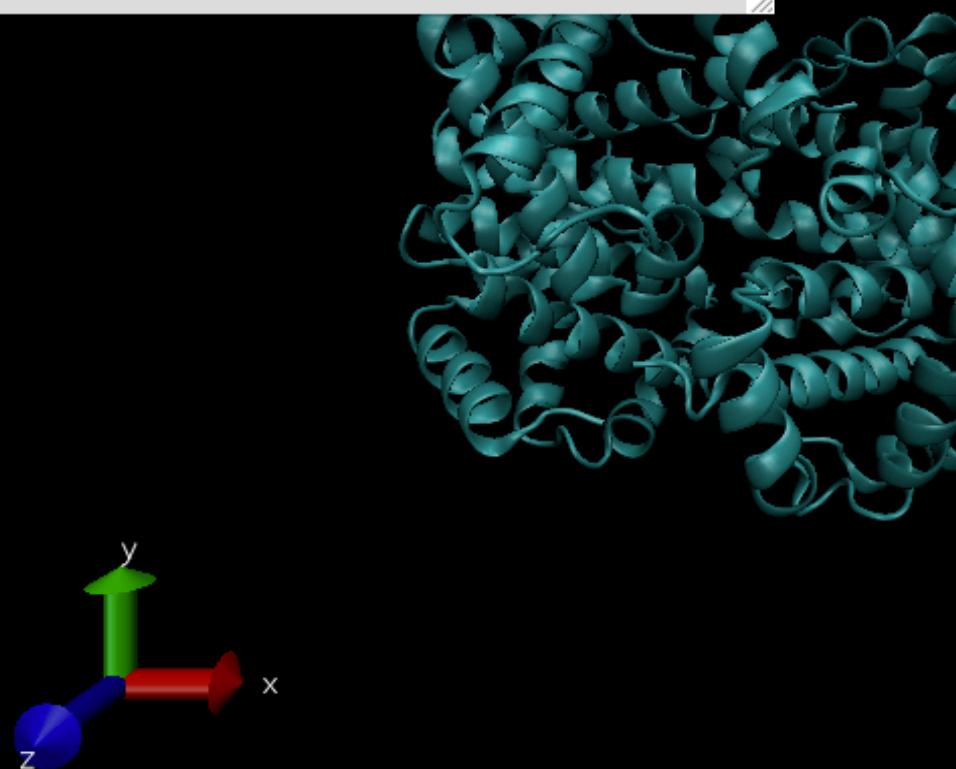
Changes Automatically Apply

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	<b>F</b>	1a3n.cif	4997	1	0

0 zoom □ Loop step □ 1 speed □ □ □



Graphical Representations

Selected Molecule  
0: 1a3n.cif

Create Rep Delete Rep

Lines Bonds DynamicBonds HBonds Points VDW CPK Licorice Polyhedra Trace Tube Ribbons NewRibbons Cartoon NewCartoon PaperChain Twister QuickSurf MSMS NanoShaper Surf VolumeSlice Isosurface FieldLines Orbital Beads Dotted Solvent

Color Selection

Name	all
------	-----

Selected Atoms

Options Trajectory Periodic Material Opaque Default

Surface Style Catmull-Rom

Resolution 10

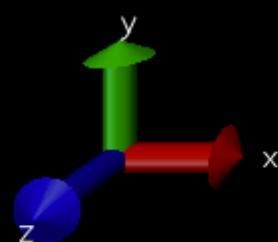
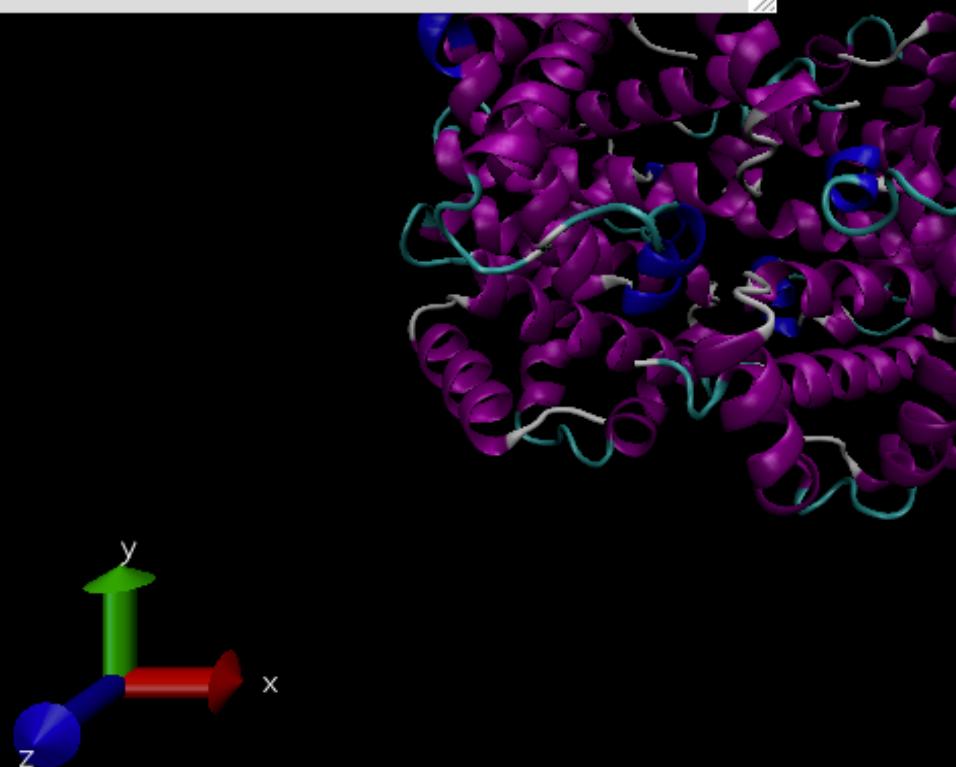
Changes Automatically Apply

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	<b>F</b>	1a3n.cif	4997	1	0

0 zoom □ Loop step ▲ 1 ▼ speed □ ▶ ▶



Graphical Representations

Selected Molecule  
0: 1a3n.cif

Create Rep Delete Rep

Style	Color	Selection
Name	Picture	all
Type		
Element		
ResName		
ResType		
ResID		
Chain		
SegName		
Conformation		
Molecule		
<b>Secondary Structure</b>		
ColorID		
Beta		
Occupancy		
Mass		
Charge		
Position		
Trajectory		
Fragment		
Index		
Backbone		
Throb		
Volume		

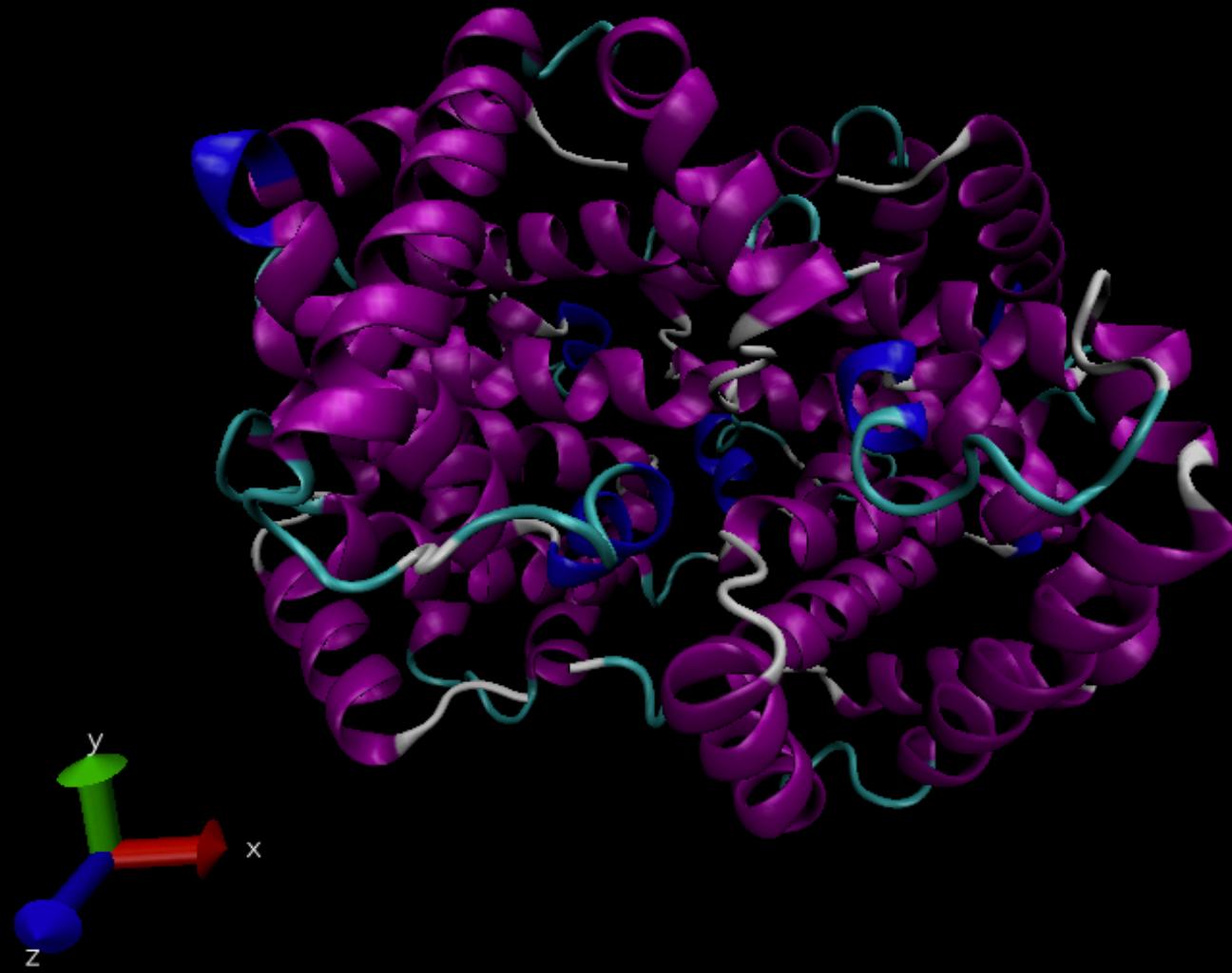
Trajectory Periodic Material Opaque ▾

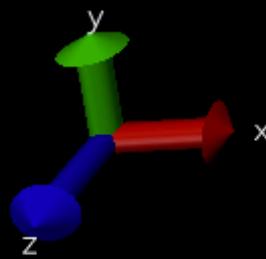
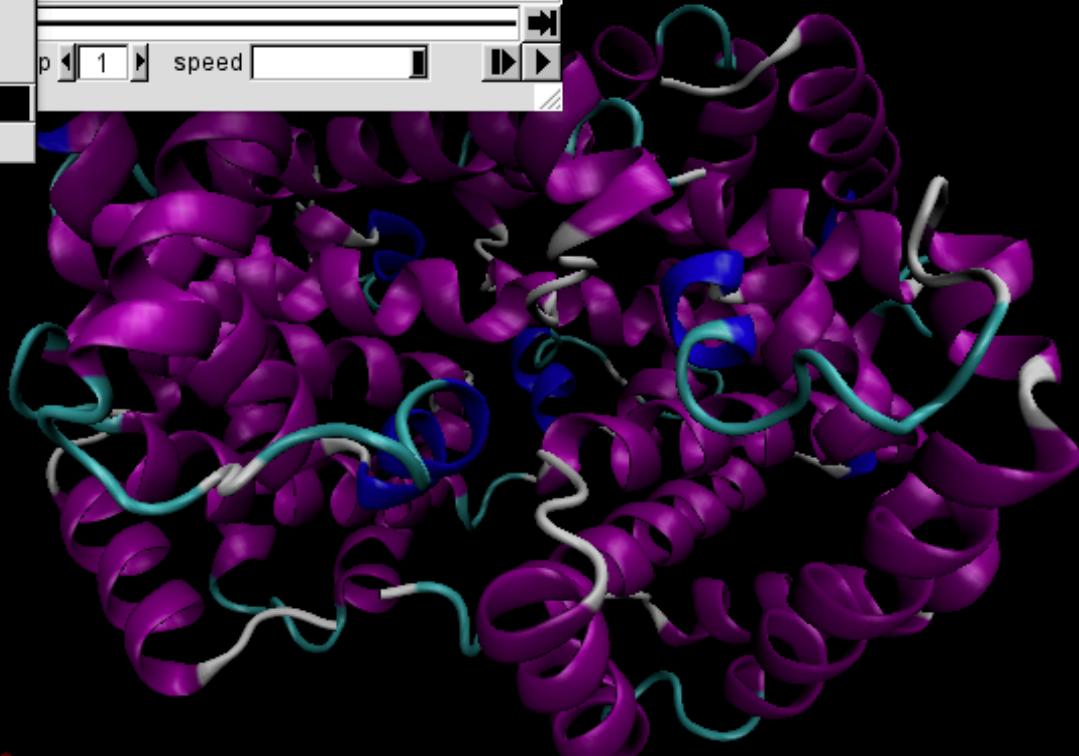
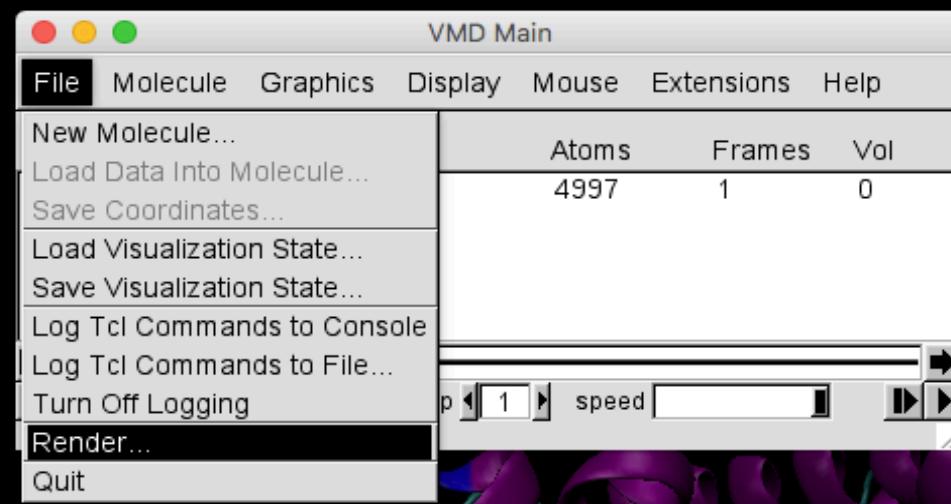
Default

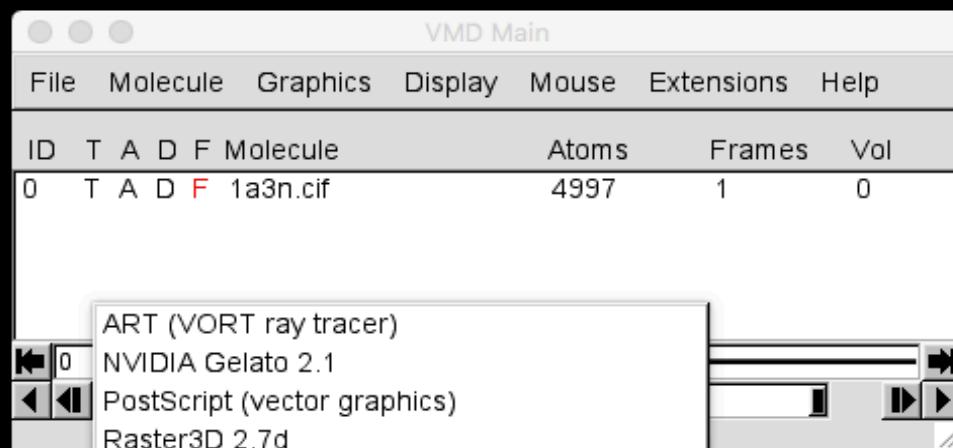
Style Catmull-Rom ▾

Resolution ▲ ▲ ▲ 10 ▲ ▾

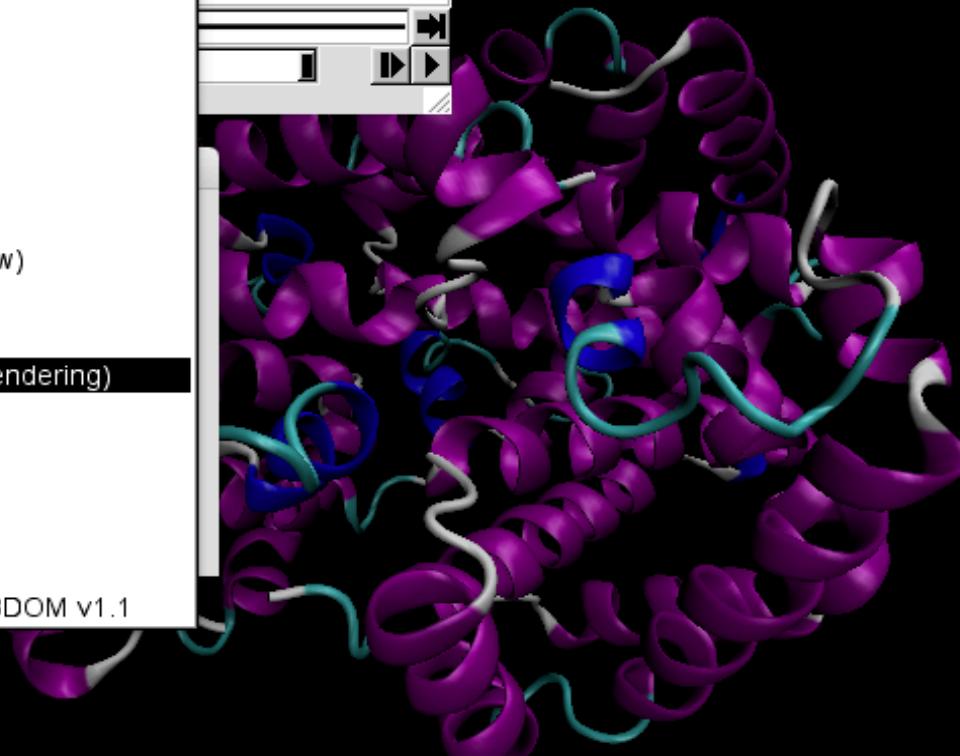
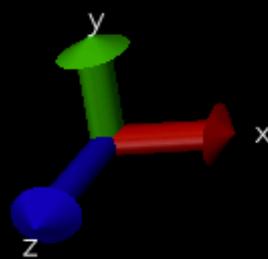
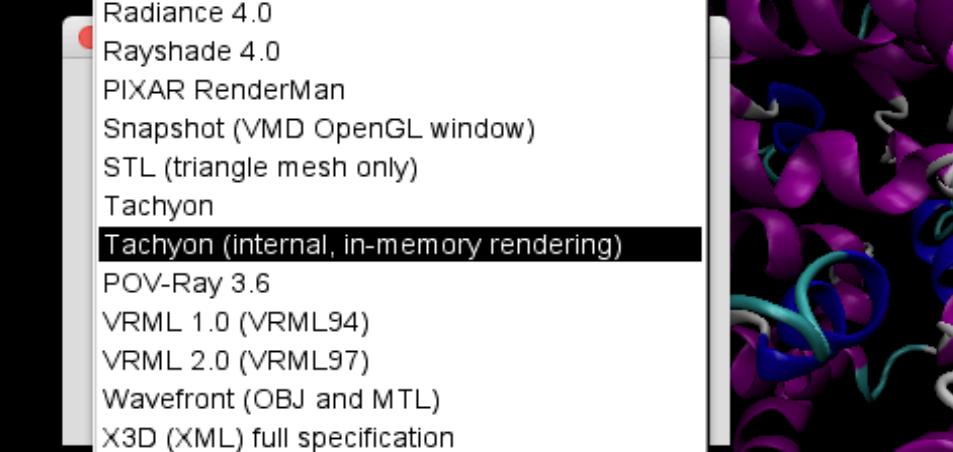
◊ Apply Changes Automatically







- ART (VORT ray tracer)
- NVIDIA Gelato 2.1
- PostScript (vector graphics)
- Raster3D 2.7d
- Radiance 4.0
- Rayshade 4.0
- PIXAR RenderMan
- Snapshot (VMD OpenGL window)
- STL (triangle mesh only)
- Tachyon
- Tachyon (internal, in-memory rendering)**
- POV-Ray 3.6
- VRML 1.0 (VRML94)
- VRML 2.0 (VRML97)
- Wavefront (OBJ and MTL)
- X3D (XML) full specification
- X3D (XML) limited subset for X3DOM v1.1



# MIT Atomic-Scale Modeling Toolkit

[https://nanohub.org/tools/ucb\\_compnano/](https://nanohub.org/tools/ucb_compnano/)

# MIT Atomic-Scale Modeling Toolkit

By Daniel Richards<sup>1</sup>, Elif Ertekin<sup>2</sup>, Jeffrey C Grossman<sup>1</sup>, David Strubbe<sup>3</sup>, Justin Riley<sup>1</sup>

1. Massachusetts Institute of Technology (MIT) 2. University of California, Berkeley 3. University of California, Merced

Tools for Atomic-Scale Modeling

Launch Tool

Version 5.31 published on 22 Oct

2017

doi:10.4231/D3VT1GS0N cite this

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Intermediate-Advanced

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Tools for Education and Research

Part of: NCN Nano-Devices for Medicine and Biology: Simulation

Tools for Education

Part of: NCN Nanomaterials:



Application:

About this Toolkit

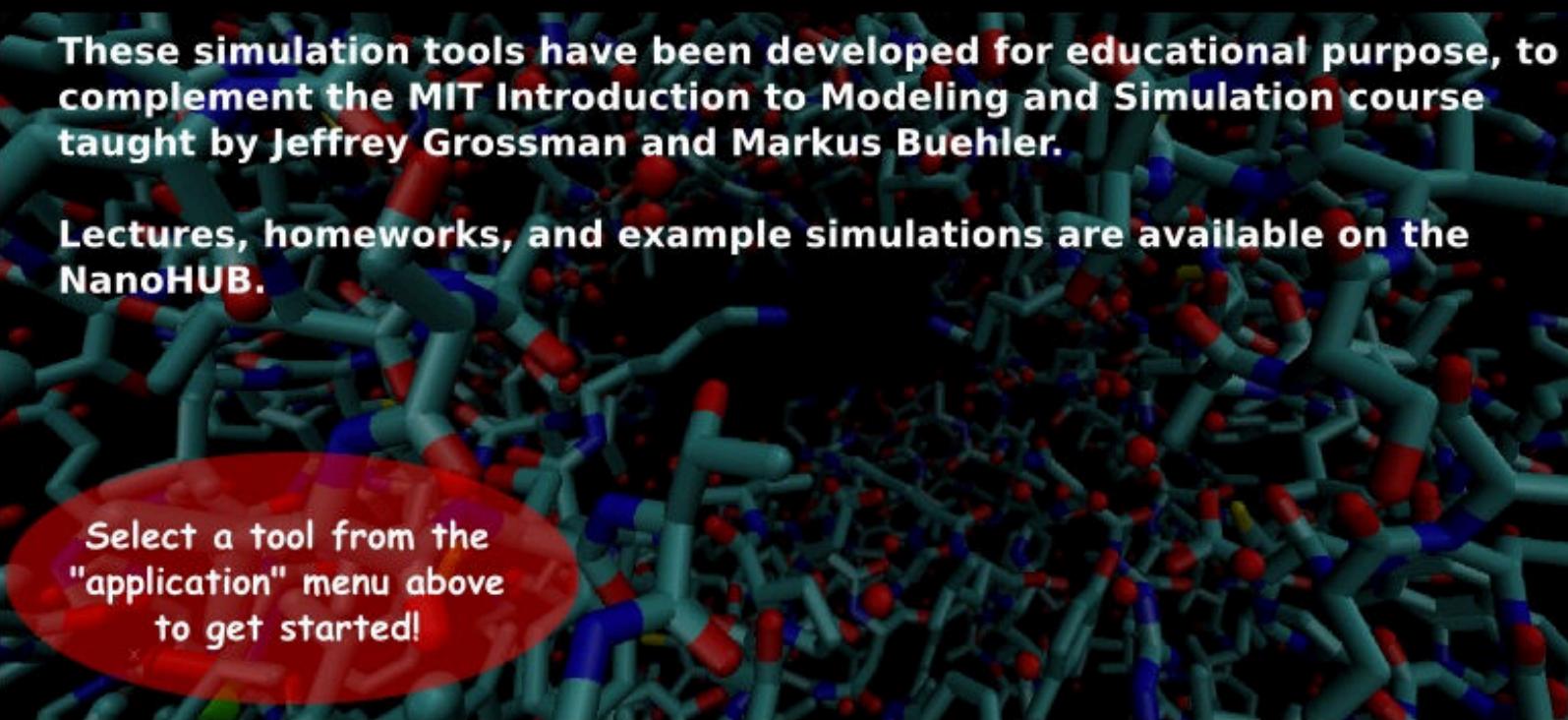


# MIT Atomic Scale Modeling Toolkit

These simulation tools have been developed for educational purpose, to complement the MIT Introduction to Modeling and Simulation course taught by Jeffrey Grossman and Markus Buehler.

Lectures, homeworks, and example simulations are available on the NanoHUB.

Select a tool from the "application" menu above to get started!



Toolkit Developers: David Strubbe, Daniel Richards, Lucas Wagner,  
Elif Ertekin, Jeffrey C. Grossman, Justin Riley



**Application:**

About this Toolkit

- About this Toolkit
- Averages and Error Bars
- Molecular Dynamics (Lennard-Jones)
- Molecular Dynamics (Carbon Nanostructures and More)
- Monte Carlo (Hard Sphere)
- Monte Carlo (Ising Model)
- Quantum Chemistry (GAMESS)
- PWSCF (Quantum Espresso)
- DFT for Solids, Surfaces, and Molecules (SIESTA)
- Quantum Monte Carlo (QWalk)

# MIT Atomic Sc

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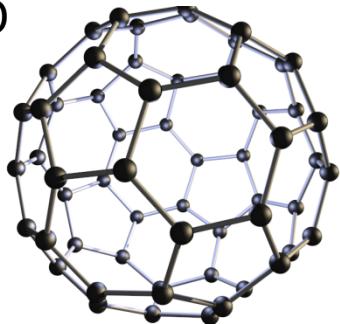
Toolkit Developers: David Strubbe, Daniel Richards, Lucas Wagner, Elif Ertekin, Jeffrey C. Grossman, Justin Riley



- Molecular Dynamics (Lennard-Jones) ←
- Molecular Dynamics (Carbon Nanostructures and more) ←
- Monte Carlo (Hard Sphere)
- Monte Carlo (Ising Model)
- Quantum Chemistry (GAMESS) ←
- PWSCF (Quantum Espresso) ←
- DFT for Solids, Surfaces and molecules (SIESTA) ←
- Quantum Monte Carlo (Qwalk)

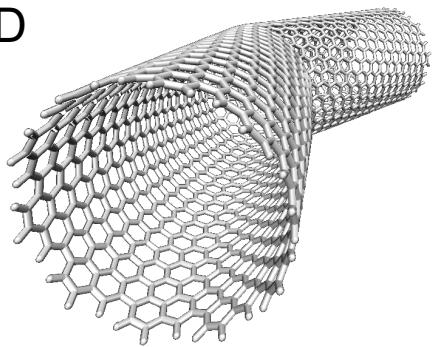
# Molecular Dynamics (Carbon nanostructures)

0D

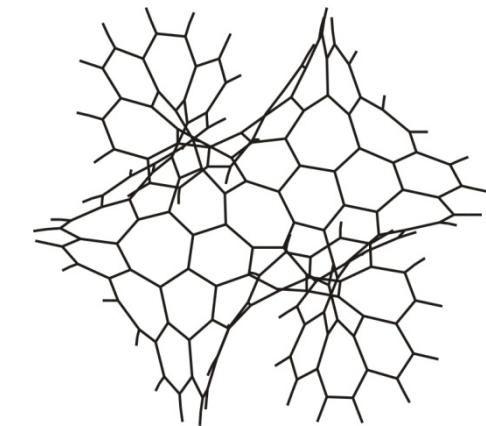


*Fullerenes*

1D

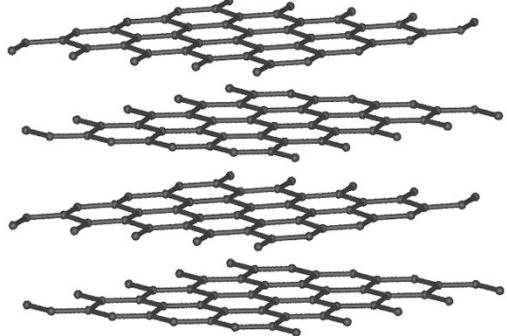


*Nanotubes*



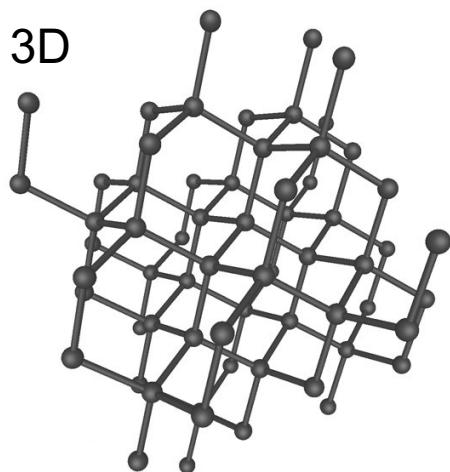
*Nano-foams*

2D

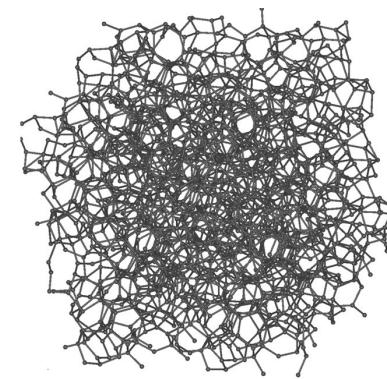


*Graphite ( $sp^2$ )*

3D



*Diamond ( $sp^3$ )*

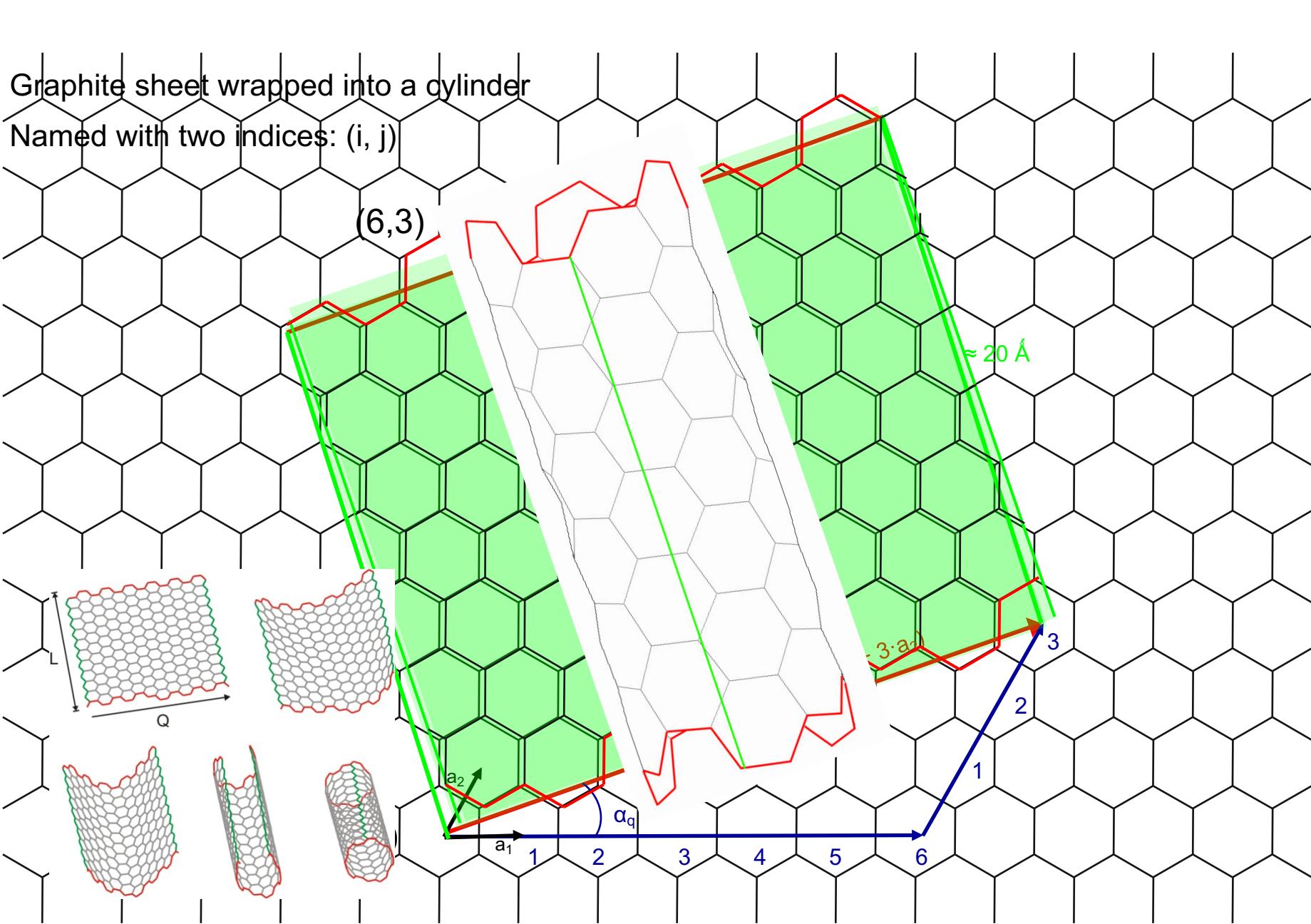


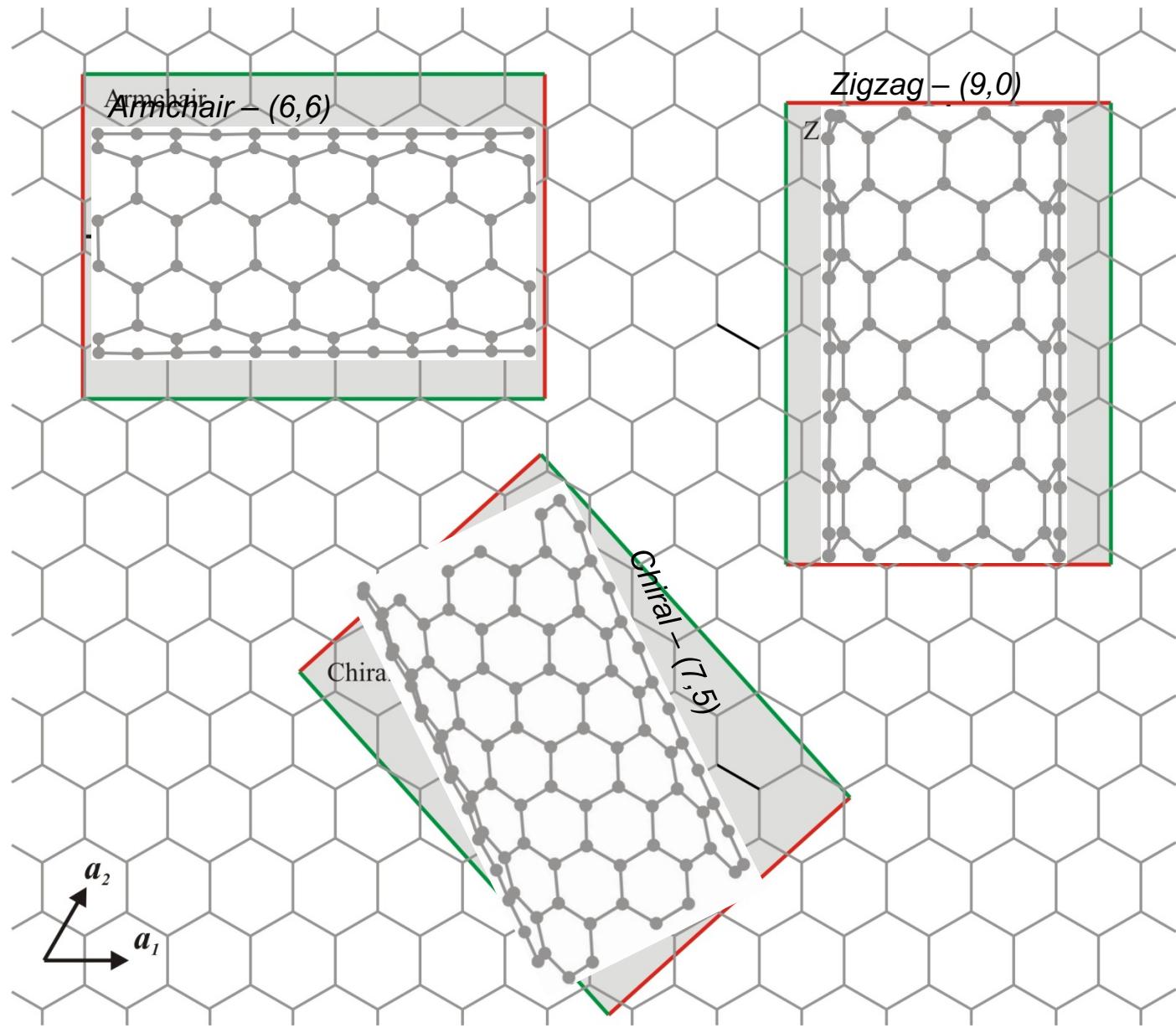
*Amofous Carbon*

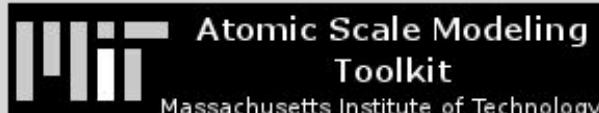
Graphite sheet wrapped into a cylinder

Named with two indices:  $(i, j)$

$(6, 3)$





**Application:**

Molecular Dynamics (Carbon Nanostructures and More)

1 Input → 2 Simulate



Choose Simulation Type: Minimize Coordinates



Choose Potential File: CH.airebo



## Minimization Options

Minimization Algorithm: Conjugate Gradient

Restart from previous run?:  noRun Jmol viewer?:  yesRun XCrySDen viewer for input structure?:  noCompute stress?:  no

## Structure and Simulation Box

XYZ Coordinates: (6,6) CNT

XYZ Coordinates: 384  
(6, 6) CNT  
c 4.06892 0.35577 0.61646  
c 3.70168 1.72636 0.61646  
c 3.34591 2.34257 1.84937  
c 2.34257 3.34591 1.84937  
c 1.72636 3.70168 0.61646  
c 0.35577 4.06892 0.61646  
c 0.35577 4.06892 1.84937

Simulate &gt;





## Application:

Molecular Dynamics (Carbon Nanostructures and More)

1 Input → 2 Simulate

Run XCrySDen viewer for input structure?:   noCompute stress?:   no

## Structure and Simulation Box

XYZ Coordinates: (6,6) CNT

New  
Upload...  
---

- (6,6) CNT
- (6,6) CNT with Stone-Wales defect
- (10,0) CNT
- (10,0) CNT with RBM
- (12,0) CNT
- (12,0) CNT with Stone-Wales defect
- (14,0) CNT
- C60 Fullerene
- C70 Fullerene
- C84 Fullerene
- C100 Fullerene
- Graphene
- Graphene with Stone-Wales defect

cell -Z (Å): **0**

Simulate &gt;

Storage (manage)



5% of 10GB



780 x 600



## Application:

Molecular Dynamics (Carbon Nanostructures and More)

1 Input → 2 Simulate



Result: LAMMPS: XYZ Coordinate Dump



```
384
Timestep: 0
C 4.06892 0.35577 0.61646
C 3.70168 1.72636 0.61646
C 3.34591 2.34257 1.84937
C 2.34257 3.34591 1.84937
C 1.72636 3.70168 0.61646
C 0.35577 4.06892 0.61646
C -0.35577 4.06892 1.84937
C -1.72636 3.70168 1.84937
C -2.34257 3.34591 0.61646
C -3.34591 2.34257 0.61646
C -3.70168 1.72636 1.84937
C -4.06892 0.35577 1.84937
C -4.06892 -0.35577 0.61646
C -3.70168 -1.72636 0.61646
C -3.34591 -2.34257 1.84937
C -2.34257 -3.34591 1.84937
C -1.72636 -3.70168 0.61646
C -0.35577 -4.06892 0.61646
C 0.35577 -4.06892 1.84937
C 1.72636 -3.70168 1.84937
```

Find: 

Select All

2 results

Clear One Clear All

Simulation = #2

&lt; Input

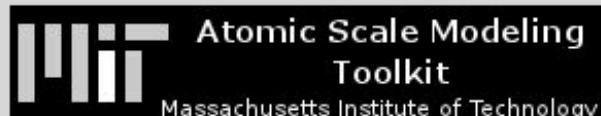
Storage (manage)



5% of 10GB



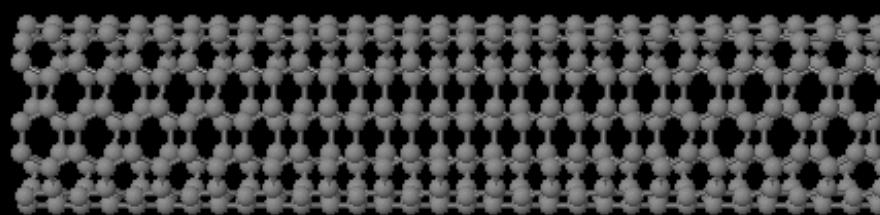
780 x 600

**Application:**

Molecular Dynamics (Carbon Nanostructures and More)



Molecular Dynamics (Carbon Nanostructures and More) Jmol x

File Edit Display View Tools MacrosHelp

776 x 404

17.7/245.4 Mb; 5/7 ms

Storage (manage)



5% of 10GB



780 x 600



## Application:

Molecular Dynamics (Carbon Nanostructures and More)

Molecular Dynamics (Carbon Nanostructures and More) Jmol X

1 Input → 2 Simulate



Result: LAMMPS: XYZ Coordinate Dump



- LAMMPS: XYZ Coordinate Dump
- LAMMPS: Final XYZ Coordinates
- LAMMPS: Log File
- LAMMPS: Input XYZ Coordinates
- LAMMPS: XSF Input
- Potential Energy
- Radial Distribution Function
- 
- Download

```
384
Times
c 4.06
c 3.70
c 3.34
c 2.34
c 1.72
c 0.39
c -0.3
c -1.
c -2.
c -3.34591 2.34257 0.61646
c -3.70168 1.72636 1.84937
c -4.06892 0.35577 1.84937
c -4.06892 -0.35577 0.61646
c -3.70168 -1.72636 0.61646
c -3.34591 -2.34257 1.84937
c -2.34257 -3.34591 1.84937
c -1.72636 -3.70168 0.61646
c -0.35577 -4.06892 0.61646
```

Find: 

Select All

2 results

Clear One Clear All

Simulation = #2

&lt; Input

Storage (manage)



5% of 10GB



780 x 600



## Application:

Molecular Dynamics (Carbon Nanostructures and More)

Molecular Dynamics (Carbon Nanostructures and More) Jmol X

1 Input → 2 Simulate



Result: LAMMPS: Log File

```
LAMMPS (31 Mar 2017)
units metal
atom_style atomic
boundary p p p
read_data lammps_data
  triclinic box = (-10 -10 0) to (10 10 39.4533) with tilt (0 0 0)
  1 by 1 by 1 MPI processor grid
  reading atoms ...
  384 atoms
pair_style lirebo 3.0
pair_coeff * * OH.lirebo C
neighbor 2.0 bin
neigh_modify every 1 delay 0
fix 1 all nve
thermo 1
thermo_style custom step etotal pe ke temp
dump 2 all xyz 1 formovie
min_style cg
minimize 1.0e-10 0.0 10000 100000
```

Find: 

Select All

2 results

Clear One Clear All

Simulation = #2

&lt; Input

Storage (manage)



5% of 10GB



780 x 600

# Molecular Dynamics (Lennard-Jones)



Application:

Molecular Dynamics (Lennard-Jones)



## Lennard-Jones Molecular Dynamics with LAMMPS

This tool performs molecular dynamics simulations in the NVE ensemble for a classical one-component system interacting via the Lennard-Jones potential:

$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

The velocity Verlet integration method is used. Periodic boundary conditions are applied for a cubic simulation box. All lengths are expressed in units of sigma. All energies (and temperature) are expressed in units of epsilon.

Simulate

new input parameters

Press Simulate to view results.

Number of particles:	32	<input type="button" value="+"/> <input type="button" value="-"/>
Temperature (units of epsilon):	1	
Box size (in units of sigma):	3	
Potential cutoff (in units of sigma):	2	
Timestep:	0.001	
Number of simulation steps:	1000	
Run Jmol viewer?:	<input checked="" type="radio"/> <input type="checkbox"/> <input type="checkbox"/>	yes



Application:

Molecular Dynamics (Lennard-Jones)

## Lennard-Jones Molecular Dynamics with LAMMPS

This tool performs molecular dynamics simulations in the NVE ensemble for a classical one-component system interacting via the Lennard-Jones potential:

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The velocity Verlet integration method is used. Periodic boundary conditions are applied for a cubic simulation box. All lengths are expressed in units of sigma. All energies (and temperature) are expressed in units of epsilon.

Simulate

new input parameters



Press Simulate to view results.

The system is isolated from changes in moles (N), volume (V), and energy (E). It corresponds to an adiabatic process with no heat exchange

Number of particles:  + -Temperature (units of epsilon): Box size (in units of sigma): Potential cutoff (in units of sigma): Timestep: Number of simulation steps: Run Jmol viewer?:   



Application:

Molecular Dynamics (Lennard-Jones)



## Lennard-Jones Molecular Dynamics with LAMMPS

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$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

**Simulate**

new input parameters

The velocity Verlet integration method is used. Periodic boundary conditions are applied for a cubic simulation box. All lengths are expressed in units of sigma. All energies (and temperature) are expressed in units of epsilon.

Number of particles:	32	<b>+</b>	<b>-</b>	
Temperature (units of epsilon):	1			
Box size (in units of sigma):	3			
Potential cutoff (in units of sigma):	2			
Timestep:	0.001			
Number of simulation steps:	1000			
Run Jmol viewer?	<input checked="" type="radio"/> <input type="checkbox"/> <input type="checkbox"/>	yes		



## Lennard Jones Interatomic Potential

strong repulsive  
forces



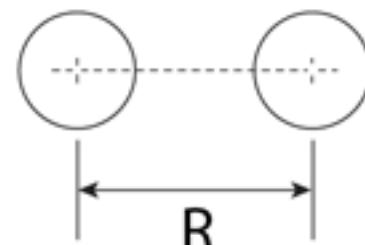
$$R < \sigma$$

separation at  
energy minimum



$$R = 1.12\sigma$$

$$U_{LJ} = 4\epsilon \left( \left( \frac{\sigma}{R} \right)^{12} - \left( \frac{\sigma}{R} \right)^6 \right)$$



$$R$$

$U_{LJ}$  (arbitrary units of energy)

$$1$$

$$0$$

$$-1$$

$$\sigma$$

$$\epsilon$$

repulsion



attraction



weak attractive  
force



$$R = 2\sigma$$



Application:

Molecular Dynamics (Lennard-Jones)



## Lennard-Jones Molecular Dynamics with LAMMPS

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Simulate

new input parameters

Number of particles:	32	<input type="button" value="+"/> <input type="button" value="-"/>
Temperature (units of epsilon):	1	
Box size (in units of sigma):	3	
Potential cutoff (in units of sigma):	2	
Timestep:	0.001	
Number of simulation steps:	1000	
Run Jmol viewer?:	<input checked="" type="radio"/> <input type="checkbox"/> <input type="checkbox"/>	yes

This is the time length  
between evaluations of  
the potential.





Application:

Molecular Dynamics (Lennard-Jones)



## Lennard-Jones Molecular Dynamics with LAMMPS

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$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

The velocity Verlet integration method is used. Periodic boundary conditions are applied for a cubic simulation box. All lengths are expressed in units of sigma. All energies (and temperature) are expressed in units of epsilon.

Simulate

new input parameters

Press Simulate to view results.

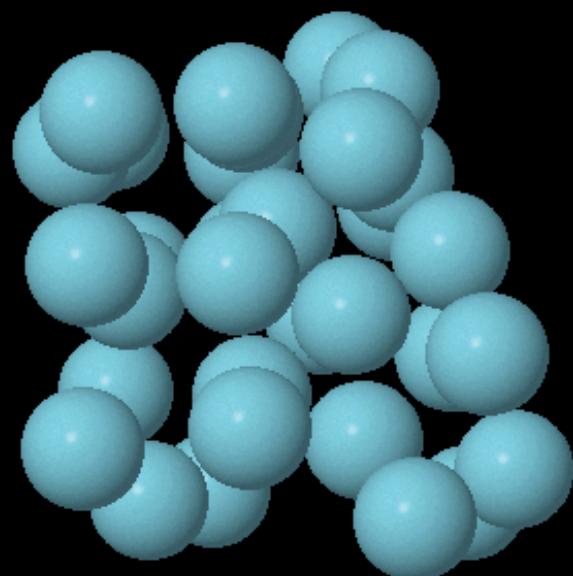
Number of particles:  + -Temperature (units of epsilon): Box size (in units of sigma): Potential cutoff (in units of sigma): Timestep: Number of simulation steps: Run Jmol viewer?:   

**MIT** Atomic Scale Modeling Toolkit  
Massachusetts Institute of Technology**Application:**

Molecular Dynamics (Lennard-Jones)

Molecular Dynamics (Lennard-Jones)

Jmol x

File Edit Display View Tools MacrosHelp

776 x 404

221.3/437.7 Mb; 11/12 ms

Storage (manage)



5% of 10GB



780 x 600



Application:

Molecular Dynamics (Lennard-Jones)

Molecular Dynamics (Lennard-Jones) Jmol

## Lennard-Jones Molecular Dynamics with LAMMPS

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The velocity Verlet integration method is used. Periodic boundary conditions are applied for a cubic simulation box. All lengths are expressed in units of sigma. All energies (and temperature) are expressed in units of epsilon.

Number of particles:  Temperature (units of epsilon): Box size (in units of sigma): Potential cutoff (in units of sigma): Timestep: Number of simulation steps: Run Jmol viewer?:   

Result: MD Coordinate Trajectory

```
32
Atoms
Ar 0 0 0
Ar 0 0 1
Ar 0 0 2
Ar 0 1 0
Ar 0 1 1
Ar 0 1 2
Ar 0 2 0
Ar 0 2 1
Ar 0 2 2
Ar 0.75 0 0
Ar 0.75 0 1
Ar 0.75 0 2
Ar 0.75 1 0
Ar 0.75 1 1
Ar 0.75 1 2
Ar 0.75 2 0
Ar 0.75 2 1
Ar 0.75 2 2
Ar 1.5 0 0
Ar 1.5 0 1
Ar 1.5 0 2
```

Find: 

1 result

See you on Monday