

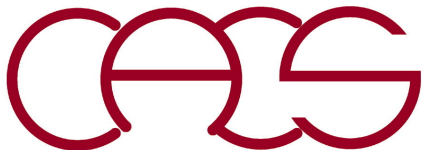
VMD & OVITO Visualization of Molecular Dynamics

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**Goal: Publication-quality image of “your” data
(gallery as final project?)**

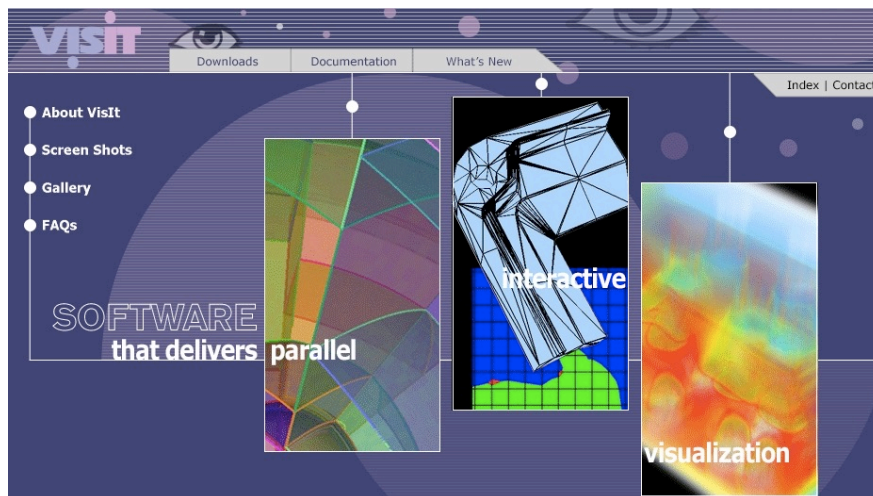
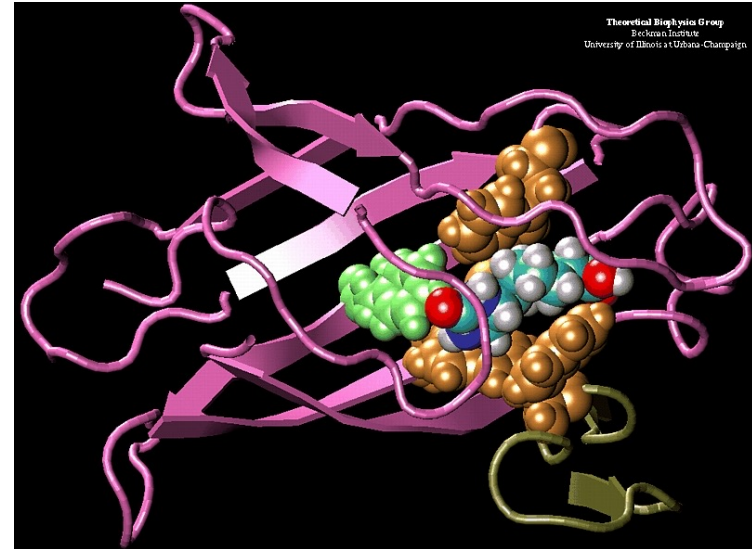


<http://www.ks.uiuc.edu/Research/vmd/gallery/>

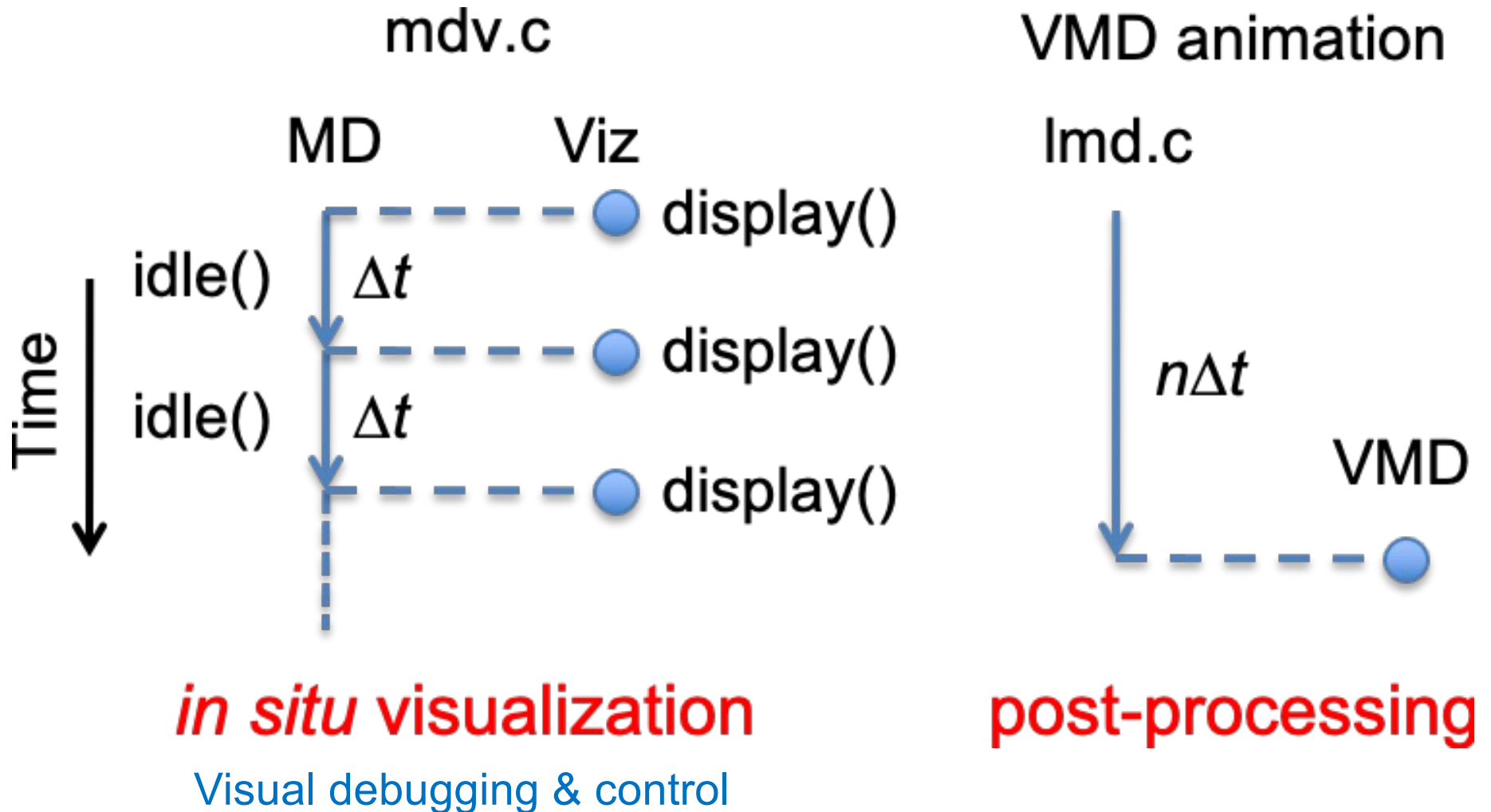


Scientific Visualization Tools

- **Atomsviewer: Billion-atom visualizer**
http://cpc.cs.qub.ac.uk/summaries/ADUM_v1_0.html
- **VMD: Molecular-dynamics data**
<http://www.ks.uiuc.edu/Research/vmd>
- **OVITO: Open visualization tool**
<https://ovito.org>
- **VisIT: General visualization system**
<https://visit.llnl.gov>
- **ParaView: General visualization system**
<http://www.paraview.org>



In Situ vs. Post-processing



In situ visualization using common visualization software?

See [B. Whitlock et al., PGM11](#)

VMD Software

- **VMD (Visual Molecular Dynamics):** Molecular visualization program developed at the University of Illinois, Urbana-Champaign.
- Downloadable for various platforms—Linux, Windows, and Mac.
- Install it on your laptop.

Version 1.9.4 LATEST ALPHA (2021-10-07) Platforms:

Latest pre-release ALPHA test version

- **Source Code**
- **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 11.x, ARM64 (64-bit "M1" Macs)** (Apple MacOS-X 11 or later)
- **MacOS 10.15, x86_64 (64-bit Intel x86_64)** (Apple MacOS-X 10.15 or later)
- **MacOS X OpenGL (32-bit Intel x86)** (Apple MacOS-X (10.10.x to 10.13.x) with hardware OpenGL (native bundle))
- **Windows 32-bit (32-bit Intel x86)** (Windows 10)
- **Windows 64-bit, CUDA, OptiX, OSPRay (64-bit Intel x86_64)** (Windows 10)

Version 1.9.3 (2016-11-30) Platforms:

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

XYZ File Format

- VMD can read various file formats such as XYZ and PDB (Protein Data Bank).
- **XYZ file format:**

Repeat the following for as many times as the number of frames (*i.e.* time steps) you would like to store

line 1: <number of atoms, N >

line 2: comment line

line 3 - $N+2$: atomic element, atom's x, y & z coordinates
(space delimited; coordinate in angstrom)

Example: a methane molecule

```
5
methane molecule (in ångströms)
C      0.000000      0.000000      0.000000
H      0.000000      0.000000      1.089000
H      1.026719      0.000000     -0.363000
H     -0.513360     -0.889165     -0.363000
H     -0.513360      0.889165     -0.363000
```

Writing an XYZ File from lmd.c

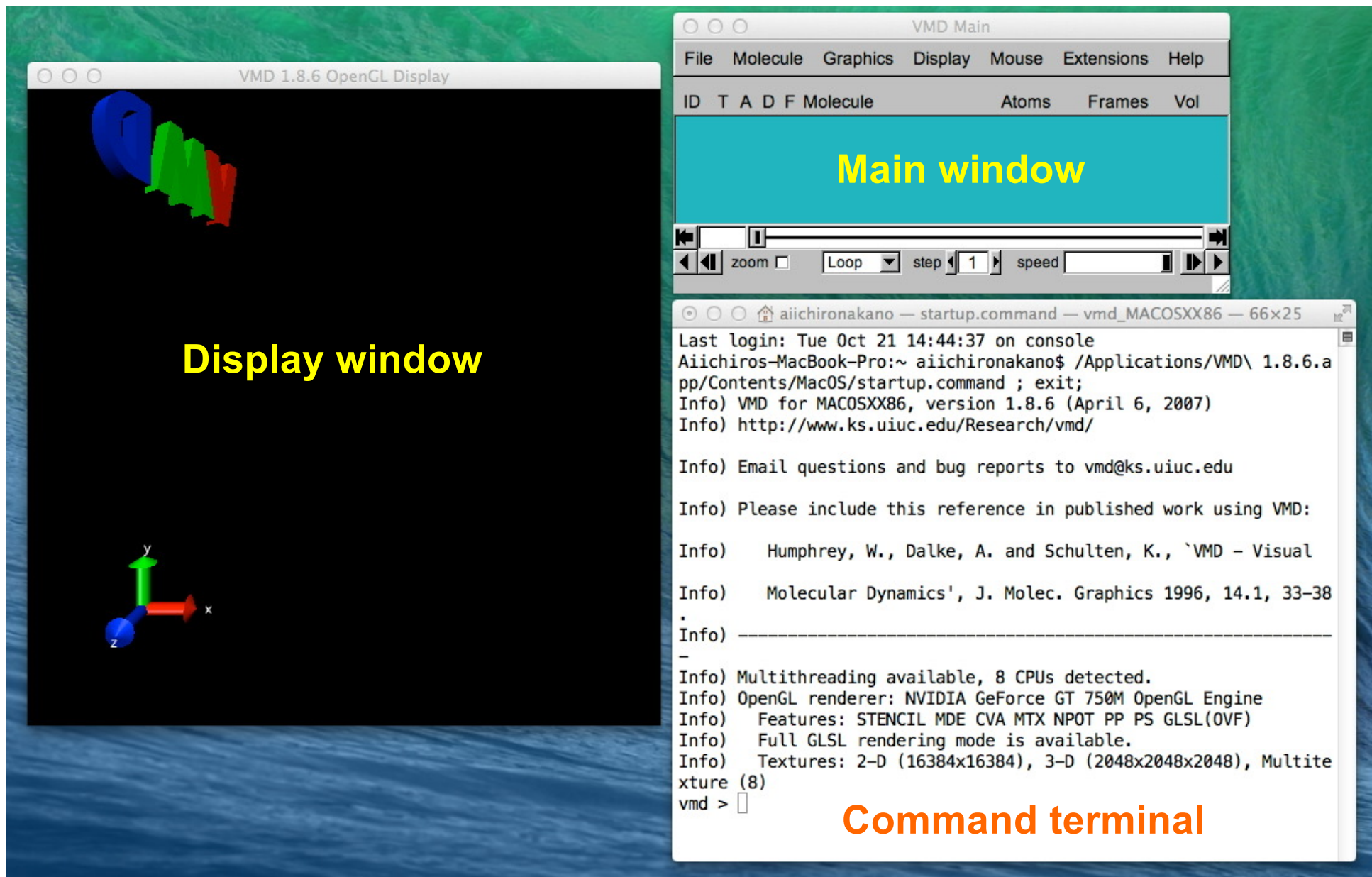
```
#define SIGMA 3.4 // Lennard-Jones length scale in angstrom
FILE *fxyz;
...
int main(int argc, char **argv) () {
    ...
    fxyz = fopen("lmd.xyz", "w");
    ... // Main MD for loop
    fclose(fxyz);
    ...
}
...
void EvalProps() {
    ...
    fprintf(fxyz, "%d\n", nAtom);
    fprintf(fxyz, "Molecular dynamics simulation of argon\n");
    for (n=0; n<nAtom; n++)
        fprintf(fxyz, "Ar %f %f %f\n", r[n][0]*SIGMA, r[n][1]*SIGMA, r[n][2]*SIGMA);
    ...
}
```

- Run the program with the following input parameters in lmd.in

```
3 3 3 // # of crystalline unit cells in the x, y & z directions
0.8 // Density in the Lennard-Jones (LJ) unit
1.0 // Temperature in the LJ unit
0.005 // Time discretization unit in the LJ unit
500 // Total # of time steps
10 // Interval between consecutive dumps to the XYZ file
```

Start VMD

- It will open 3 windows



The screenshot displays three windows from the VMD (Visual Molecular Dynamics) software interface:

- Display window:** A window titled "VMD 1.8.6 OpenGL Display" showing a 3D molecular model with blue, green, and red components. A 3D coordinate system with x, y, and z axes is visible at the bottom.
- Main window:** A window titled "VMD Main" with a menu bar (File, Molecule, Graphics, Display, Mouse, Extensions, Help) and a table with columns: ID, T, A, D, F, Molecule, Atoms, Frames, Vol. The main area contains the text "Main window" in yellow.
- Command terminal:** A terminal window titled "aiichironakano — startup.command — vmd_MACOSXX86 — 66x25" showing the startup command and output:

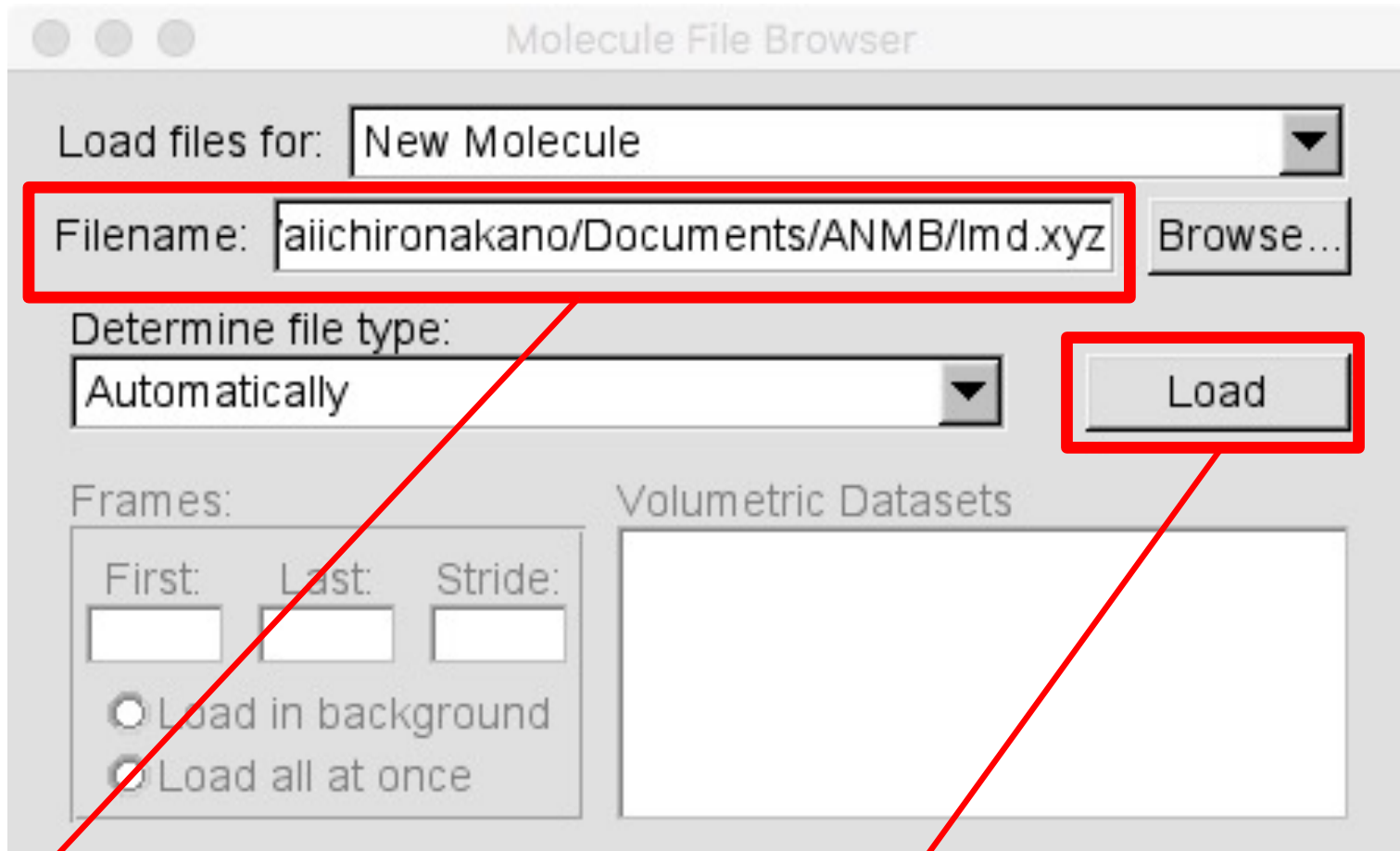
```
Last login: Tue Oct 21 14:44:37 on console
Aiichiros-MacBook-Pro:~ aiichironakano$ /Applications/VMD\ 1.8.6.app/Contents/MacOS/startup.command ; exit;
Info) VMD for MacOSXX86, version 1.8.6 (April 6, 2007)
Info) http://www.ks.uiuc.edu/Research/vmd/

Info) Email questions and bug reports to vmd@ks.uiuc.edu

Info) Please include this reference in published work using VMD:
Info)   Humphrey, W., Dalke, A. and Schulten, K., `VMD - Visual
Info)   Molecular Dynamics', J. Molec. Graphics 1996, 14.1, 33-38
Info)   -----
Info)   -
Info) Multithreading available, 8 CPUs detected.
Info) OpenGL renderer: NVIDIA GeForce GT 750M OpenGL Engine
Info)   Features: STENCIL MDE CVA MTX NPOT PP PS GLSL(OVF)
Info)   Full GLSL rendering mode is available.
Info)   Textures: 2-D (16384x16384), 3-D (2048x2048x2048), Multitexture (8)
vmd > 
```

Load the MD-Trajectory XYZ File

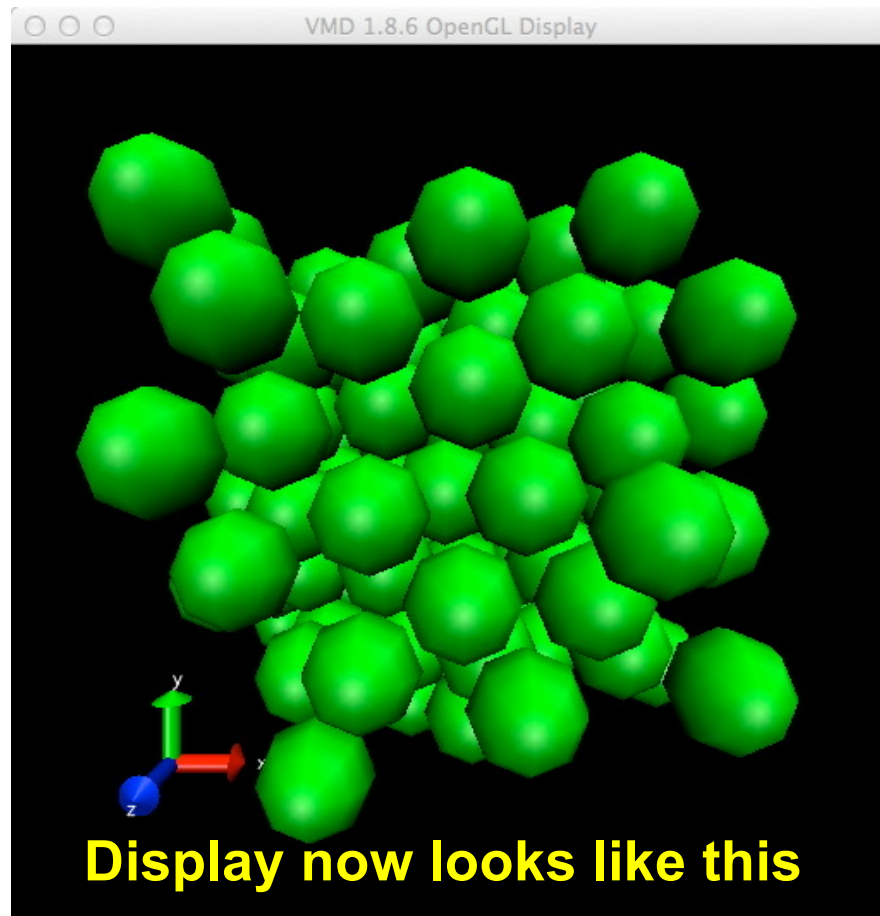
- In the File menu in the VMD main window, select New Molecule; the following new window will open.



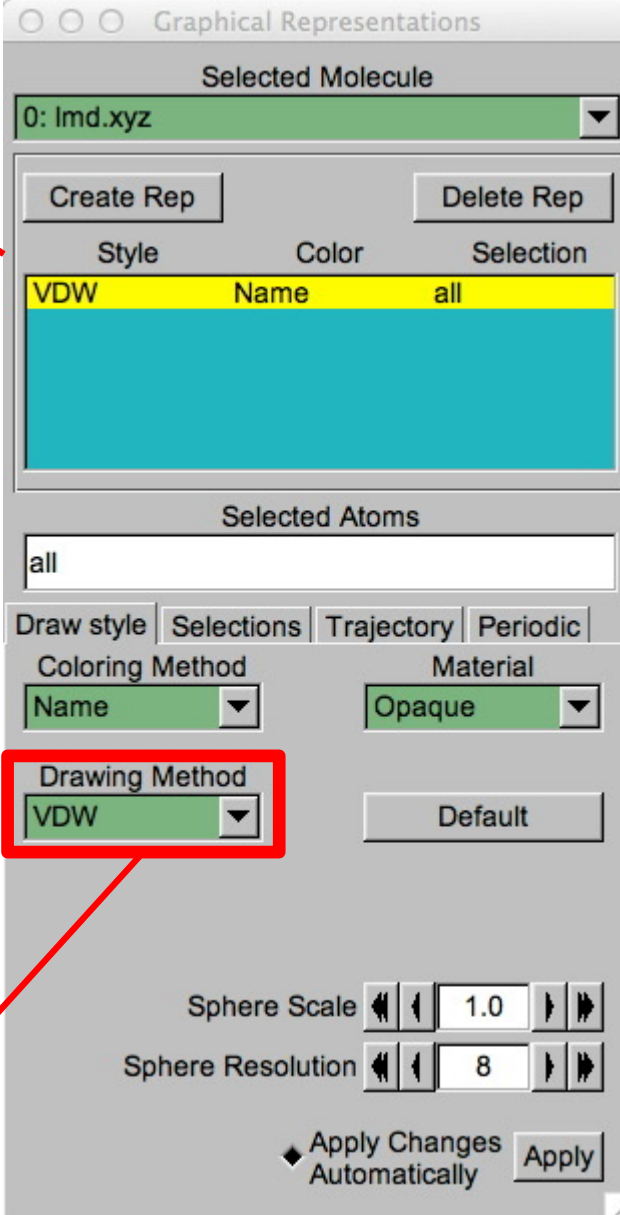
- Drag and drop the XYZ file you have created in the Filename field (or press the browse button to locate the file).
- Click the Load button to load the file.

Choose the Graphic Representation

- In the Graphics menu in the VMD main window, select Representations; the following new window will open.



- In the Drawing Method menu, choose the VDW (van der Waals radius) representation.



Graphical Representations

Selected Molecule
0: lmd.xyz

Create Rep Delete Rep

Style	Color	Selection
VDW	Name	all

Selected Atoms
all

Draw style Selections Trajectory Periodic

Coloring Method
Name

Material
Opaque

Drawing Method
VDW

Default

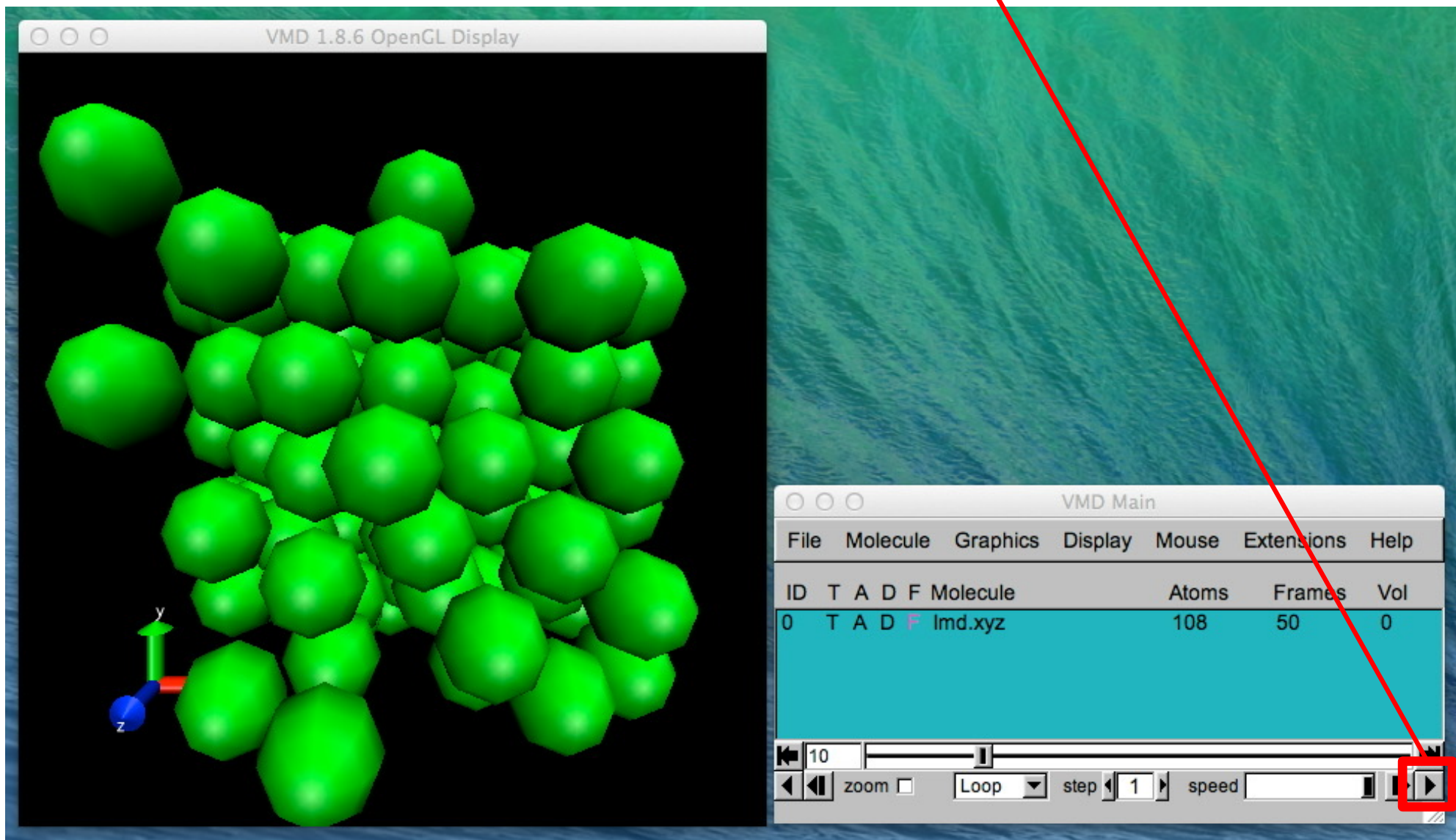
Sphere Scale 1.0

Sphere Resolution 8

Apply Changes Automatically Apply

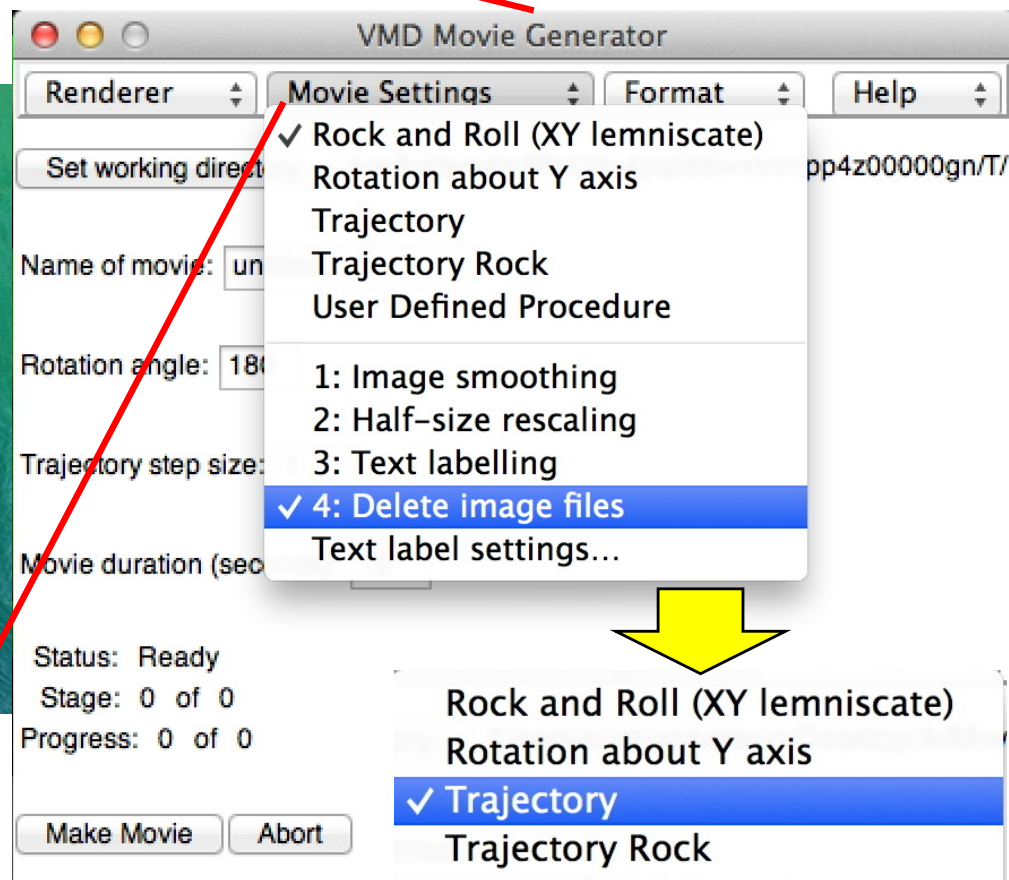
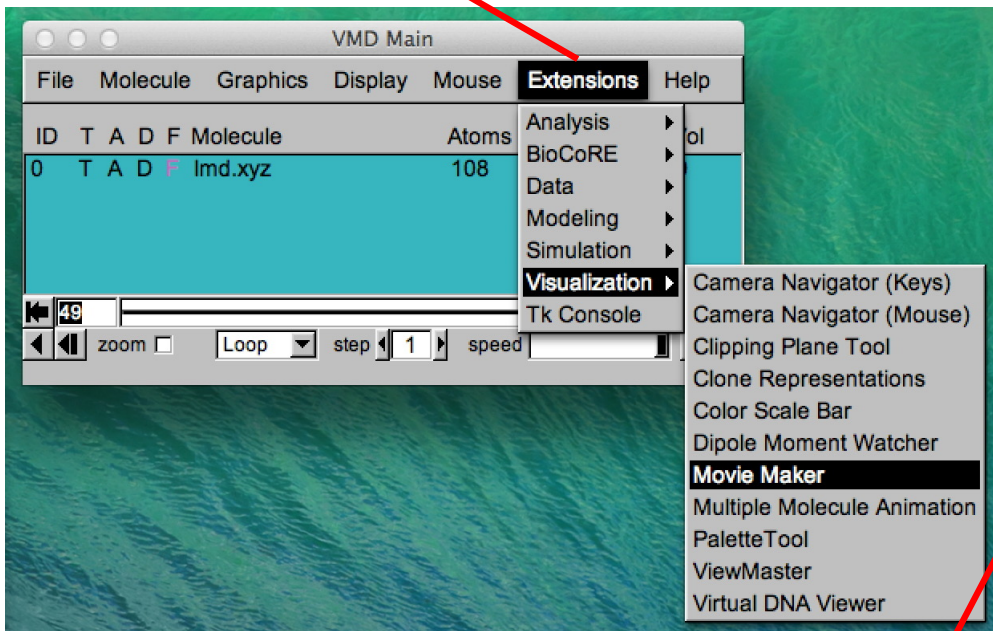
Animation

- Click the play button in the VMD main window to play the movie.

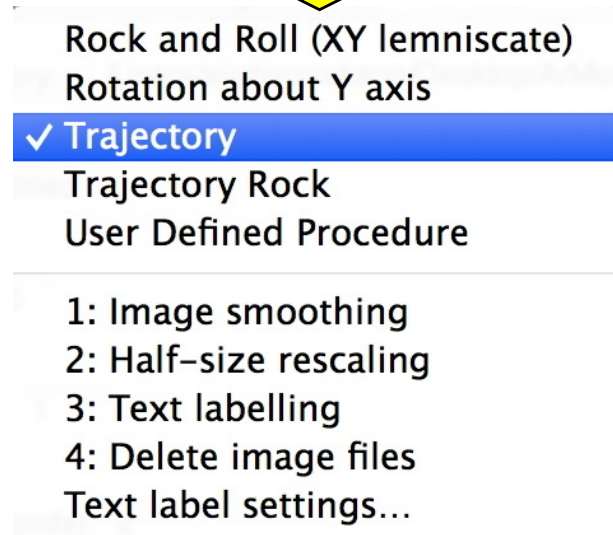


Optional: Creating a Movie File (1)

- Choose the Extensions → Visualization → Movie Maker menu; this will open a VMD Movie Generator window.

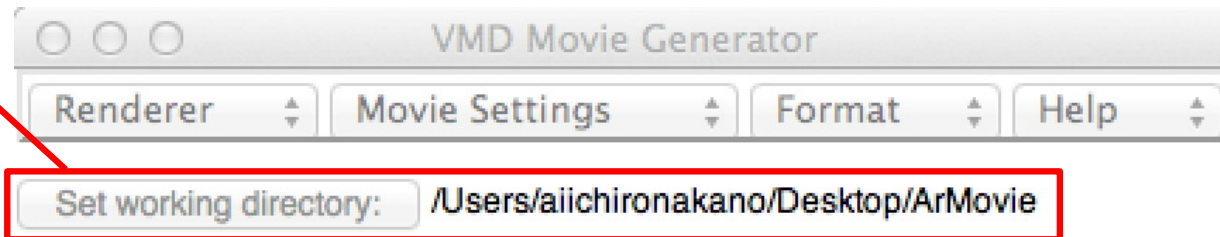


- Unclick (1) the “Rock and Roll” & (2) “Delete image files” options, while clicking the “Trajectory” option, in the “Movie Settings” menu.



Optional: Creating a Movie File (2)

- Choose a directory, in which a sequence of image files will be stored, using the “Set working directory” field.



Name of movie:

Rotation angle:

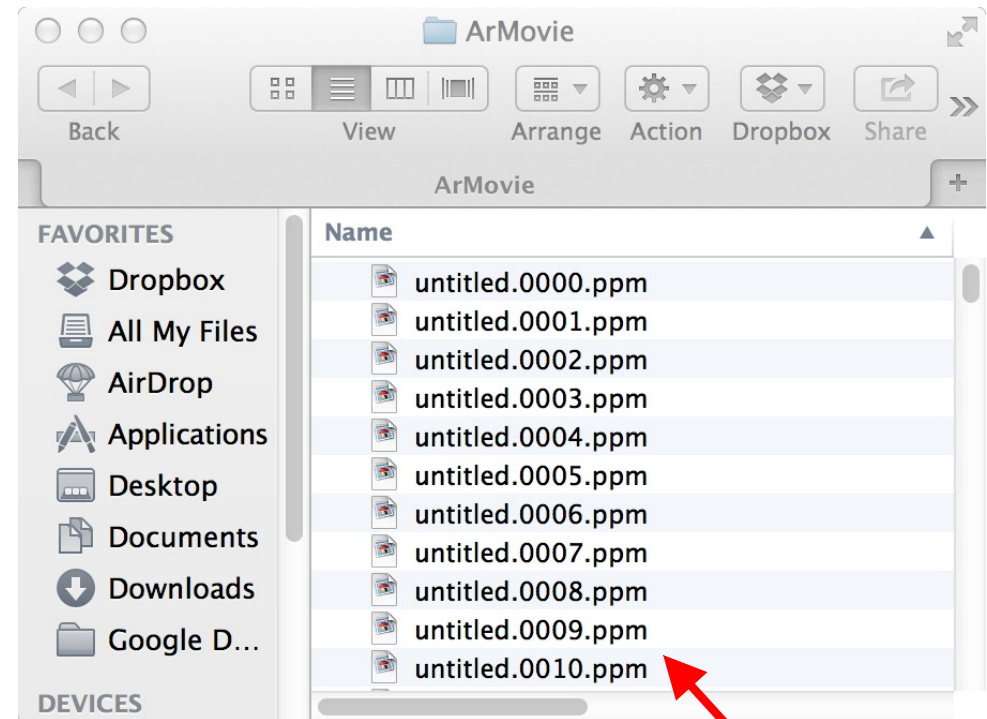
Trajectory step size:

Movie duration (seconds):

Status: Ready

Stage: 0 of 0

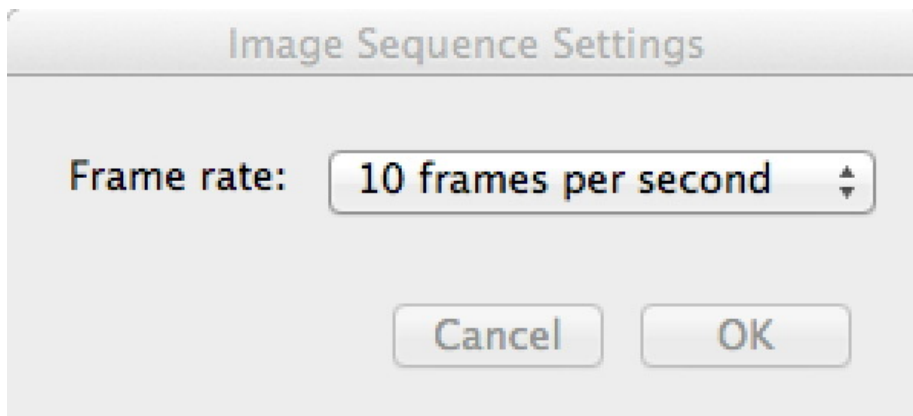
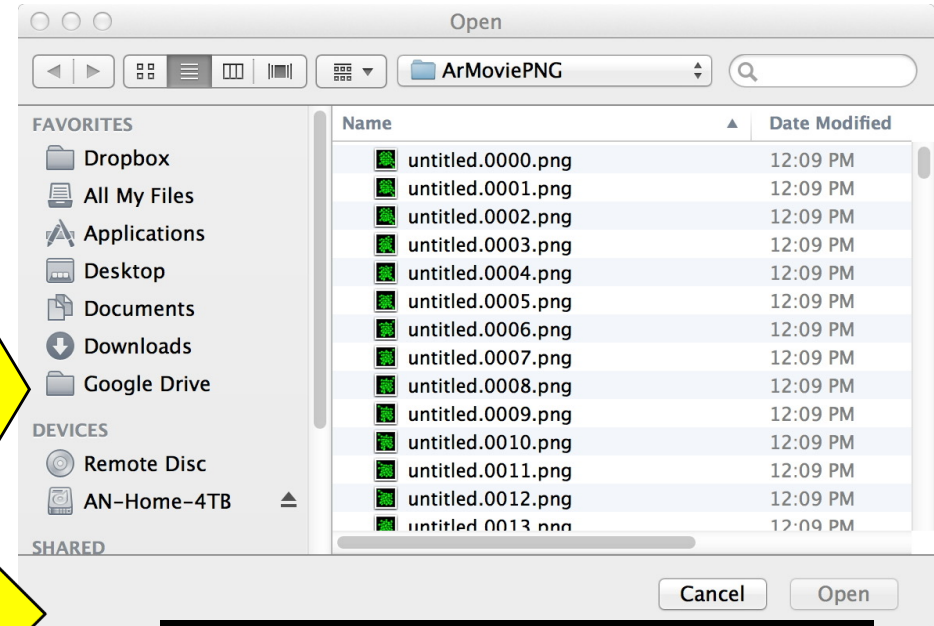
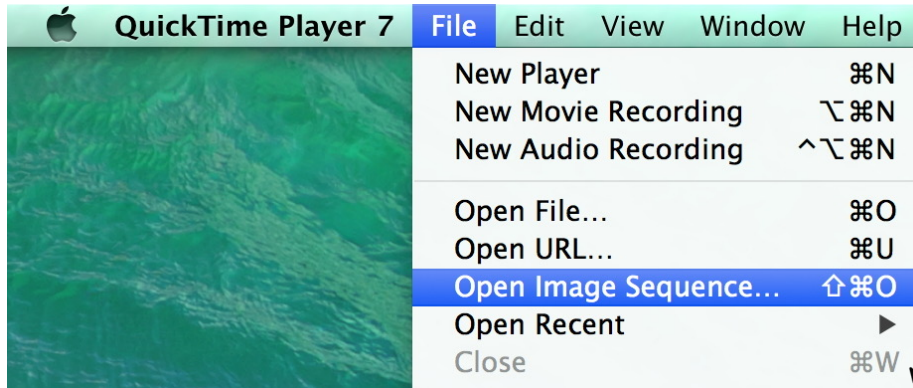
Progress: 0 of 0



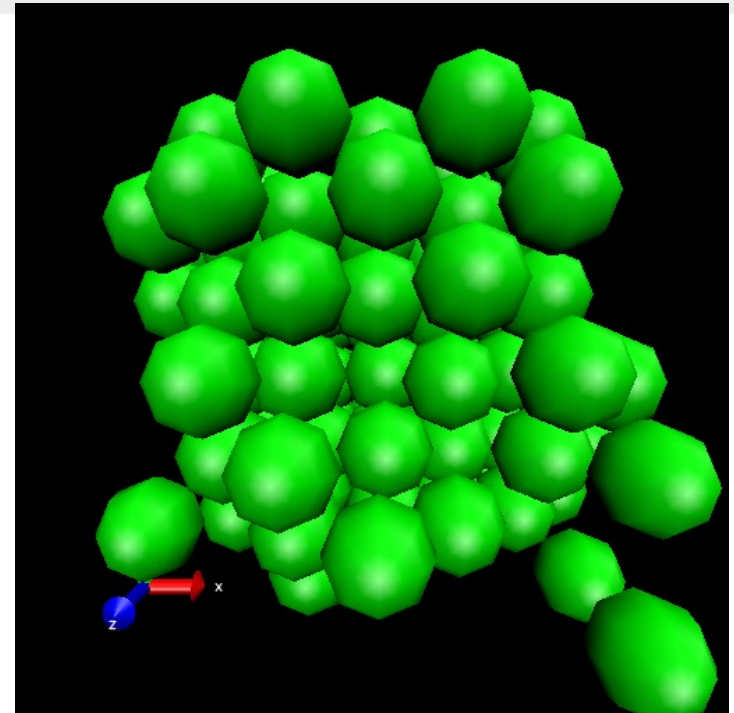
- Click the “Make Movie” button; you will find image files in the directory.

Optional: Creating a Movie File (3)

- Use a software such as QuickTime Player to convert the image sequence to a movie file.

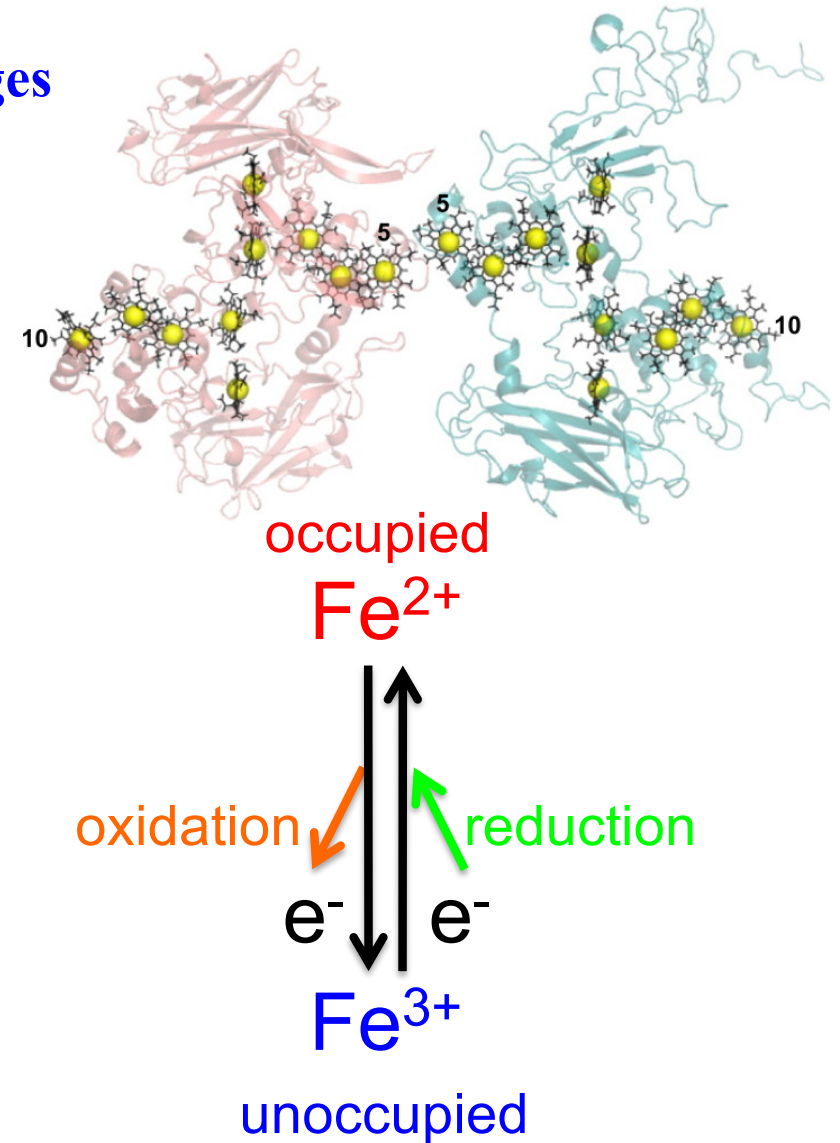
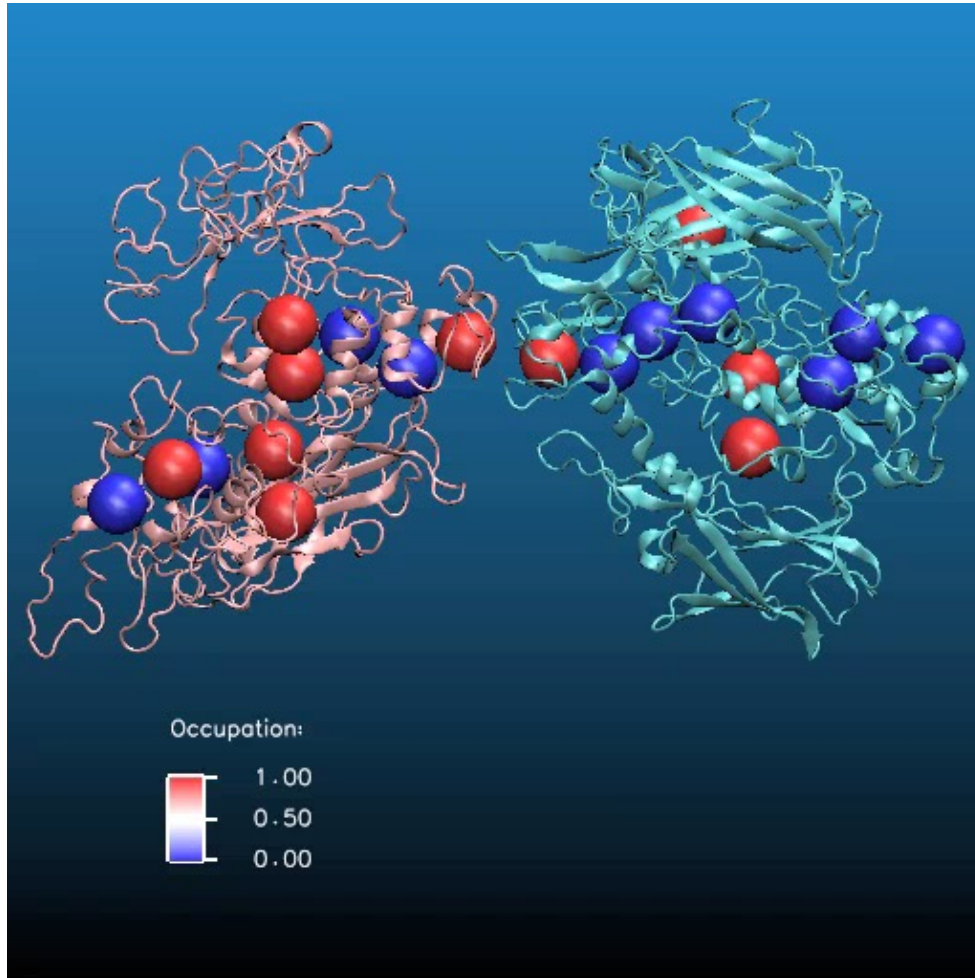


- Before this step, we have converted the PPM (portable pixmap) image files created by VMD to PNG (portable network graphics) image files that QuickTime Player can read, using the GraphicsConverter software.



Dynamic Coloring

- In VMD, USER fields in the TRAJECTORY data category can be animated as color changes according to one of the built-in color scales



Scripting in VMD

- VMD allows **Tcl** scripting language for user to control visualization
- Go to File → New Molecule menus → load complex16 pdb—cytochrome (MtrF-OmcA) dimer data—in Filename textbox
 - > Graphics → Representations → choose NewCartoon in Drawing Method
- Extensions → Tk Console → type the following commands in console

```
%cd csci596-as07      Absolute path that contains Tcl script named userb.tcl
%source userb.tcl
```
- It loads FeOcc.pdb—time series of Fe positions & their occupations (0 or 1)
 - > Graphics → Representations (make sure Selected Molecule is FeOcc.pdb)
 - >> Drawing Method → VDW; set sphere scale to be 4.0
 - >> Coloring Method → Trajectory → User → User
 - > Graphics → Colors → Color scale → Method: BWR
- Click play button in VMD main window for animation

Tcl Script

- In FeOcc.pdb file, “beta” value in the last column is customized to represent electron occupation (0 or 1) for each Fe atom; Tcl script FeOcc.pdb transfers it to “user” field used for VMD coloring

<https://aiichironakano.github.io/cs596/src/viz/userb.tcl>

```
mol new FeOcc.pdb waitfor all
set all [atomselect top all]
set frame 0
set in [open FeOcc.pdb r]
set beta {}
while { [gets $in line] != -1 } {
  switch -- [string range $line 0 3] {
    END {
      $all frame $frame
      $all set user $beta
      set beta {}
      incr frame
    }
    HETA -
    ATOM {
      lappend beta [expr [string range $line 60 65]]
    }
  }
}
```

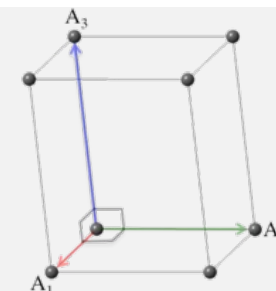
Find more examples: https://www.ks.uiuc.edu/Research/vmd/script_library/

Publish your Tcl script as VMD plugin: I. Balabin et al., [*J. Comput. Chem.* **33**, 906 \('12\)](#)

Gaussian Cube File Format

- **Cube file format:** Describes volumetric data (*e.g.*, electronic wave function or charge density) as well as atom positions

```
<header>
<comment>
 24   0.000000   0.000000   0.000000 // # atoms & origin
 63   0.198958   0.000000   0.000000 // # of voxels 1st axis
 63  -0.099479   0.172302   0.000000 //                2nd
189   0.000000   0.000000   0.194054 //                3rd
 42   0.000000  -0.000013   3.618358   4.860106 // atomic #, nuclear charge,
 42   0.000000   6.267168   3.618358   4.860106 // & atomic position vector
...
0.29654E-04  0.25769E-04  0.20454E-04  0.15027E-04  0.98477E-05  0.53243E-05
... // volumetric data (see the code below)
```



```
for (ix=0;ix<NX;ix++) {
  for (iy=0;iy<NY;iy++) {
    for (iz=0;iz<NZ;iz++) {
      printf("%g ",data[ix][iy][iz]); if (iz % 6 == 5) printf("\n");
    } printf("\n");
  }
}
```

Isosurface Rendering

- Load a cube file <https://aiichironakano.github.io/cs596/src/viz/MoSe2-hole.cube>
- Draw atoms using VDW representation & bond between atoms using dynamic-bond representation (adjust sphere radius & bond cutoff)
- Draw the volumetric data using isosurface representation (adjust isovalue)

The image displays three sequential screenshots of the 'Graphical Representations' window, illustrating the configuration of different rendering methods for a molecule (MoSe2-hole.cube). Red arrows indicate the progression from left to right.

First Screenshot (Left): The 'Selected Molecule' is '0: MoSe2-hole.cube'. The 'Style' table shows 'VDW' with 'Name' and 'Selection' 'all'. The 'Drawing Method' is set to 'VDW'. The 'Sphere Scale' is set to 0.3.

Style	Color	Selection
VDW	Name	all

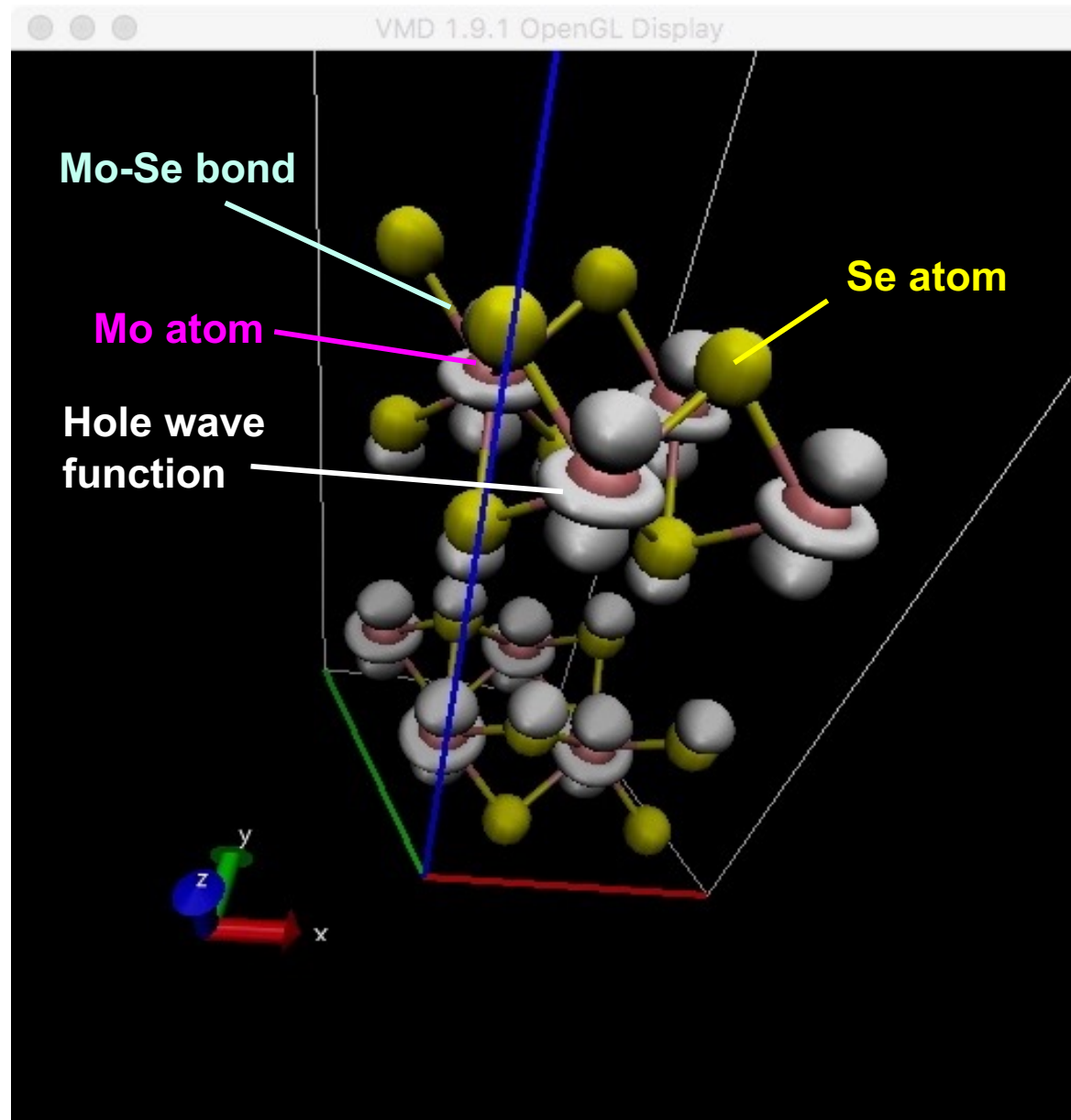
Second Screenshot (Middle): The 'Style' table now includes 'DynamicBonds' with 'Name' and 'Selection' 'all'. The 'Drawing Method' is set to 'DynamicBonds'. The 'Distance Cutoff' is set to 2.6.

Style	Color	Selection
VDW	Name	all
DynamicBonds	Name	all

Third Screenshot (Right): The 'Style' table now includes 'Isosurface' with 'Name' and 'Selection' '<volume>'. The 'Drawing Method' is set to 'Isosurface'. The 'Isovalue' is set to 0.001088. The 'Draw' dropdown is set to 'Solid Surface'.

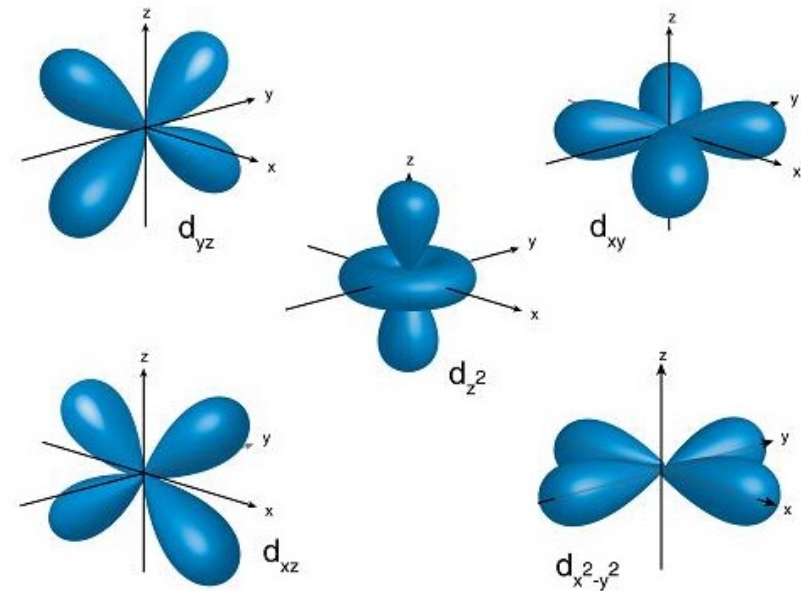
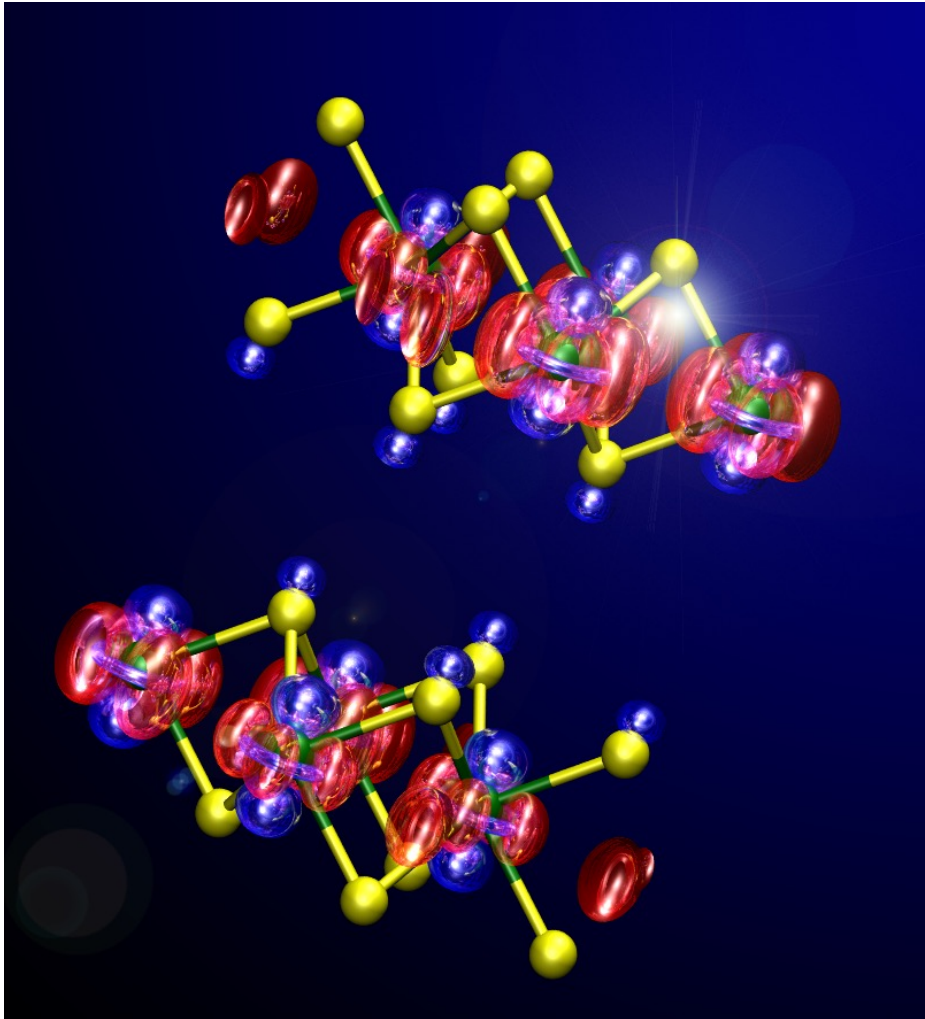
Style	Color	Selection
VDW	Name	all
DynamicBonds	Name	all
Isosurface	Name	<volume>

Isosurface Rendering



Wave Functions in MoSe₂ Bilayer

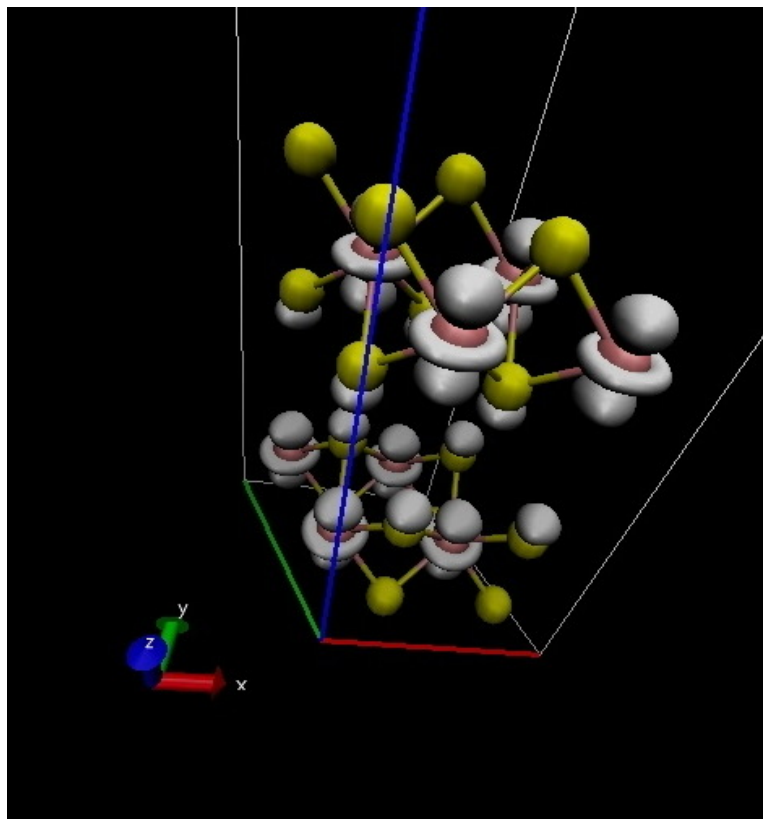
- Highest occupied states (blue) are d_{z^2} -like
- Lowest unoccupied states (red) are d_{xy} -like



**Electron
Hole**

**Try a different
rendering method:
File →
render →
tachyon internal**

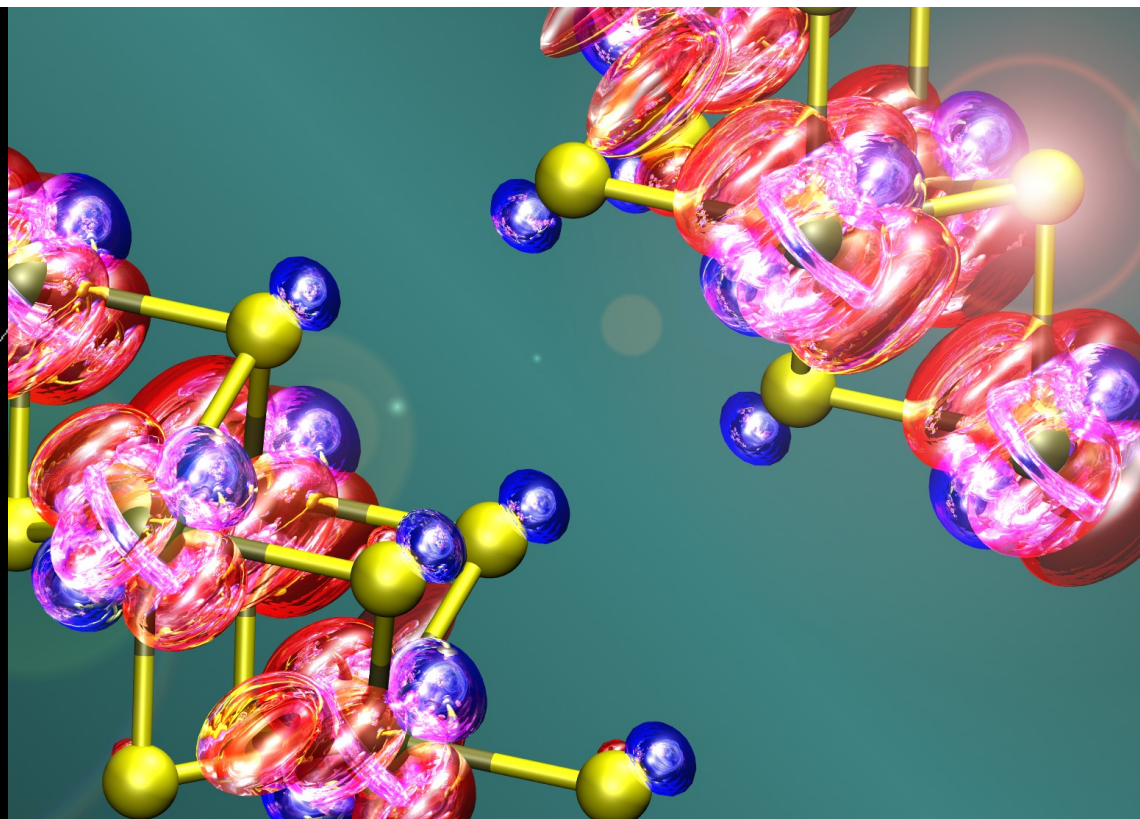
Beautify in One Hour?



Before

Default VMD rendering

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



After

Enhanced with POV-ray ray tracer

<http://www.povray.org>

Try: File → render → POV-Ray

M.F. Lin *et al.*, *Nature Commun.* **8**, 1745 ('17)

OVITO Software

- **OVITO (Open Visualization Tool): Scientific visualization and analysis software for atomistic & particle simulation data.**

A. Stukowski, “Visualization and analysis of atomistic simulation data with OVITO – the Open Visualization Tool,” *Modelling Simul. Mater. Sci. Eng.* **18**, 015012 ('10)

- **Downloadable for various platforms—Linux, Windows, and Mac.**
- **Install it on your laptop.**
<https://www.ovito.org>

OVITO Basic

Open-source software – limited feature set

Version 3.9.2 – 31 Aug, 2023

OVITO Pro

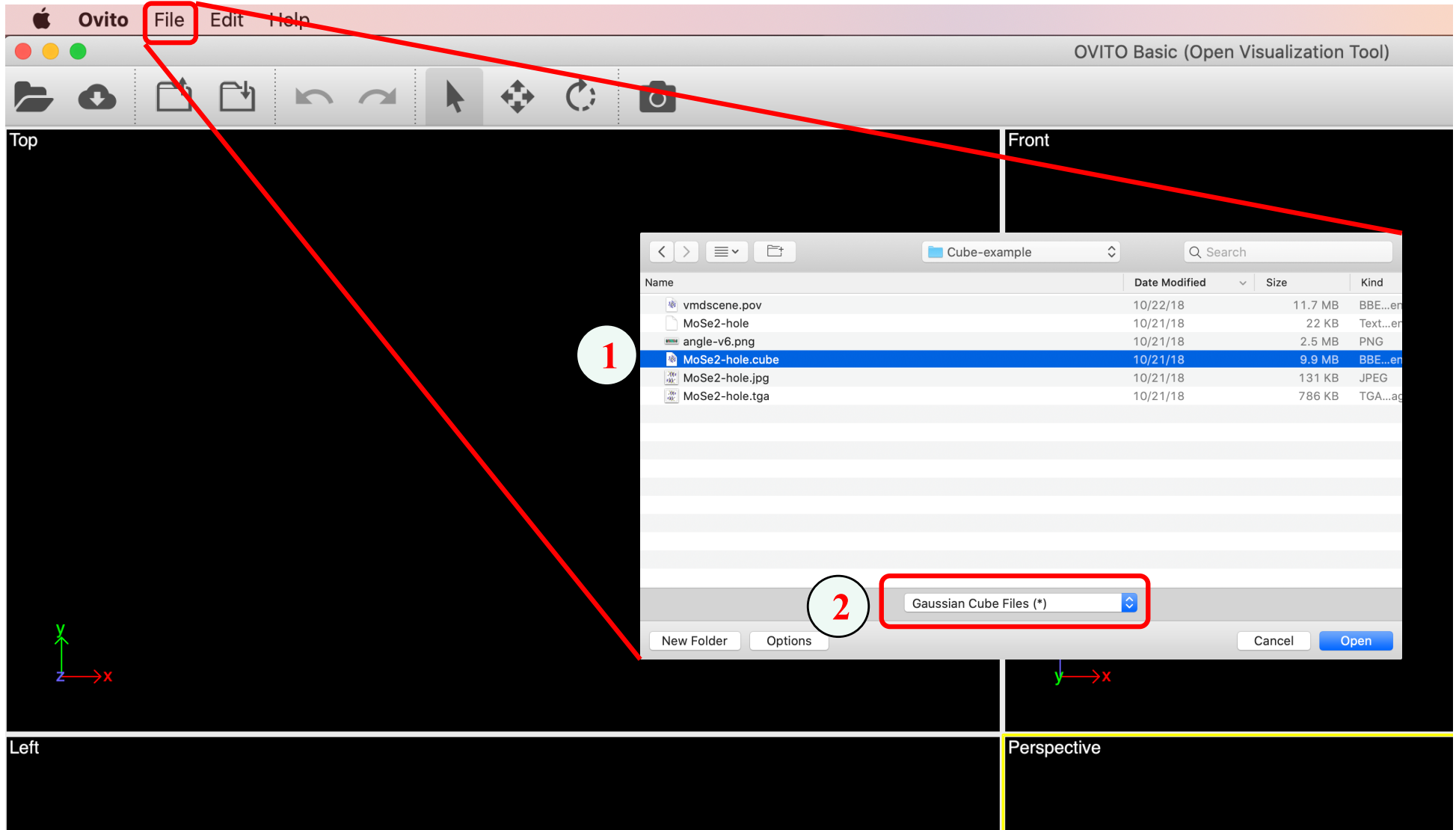
Professional version – full functionality

Version 3.9.2 – 31 Aug, 2023

Unfortunately, the isosurface feature is no longer free!

Isosurface Rendering Using OVITO

- Start OVITO & choose the “file” then “load file” menu
- (1) Load a cube file <https://aiichironakano.github.io/cs596/src/viz/MoSe2-hole.cube>,
(2) specifying “Gaussian Cube Files” format



Isosurface Rendering Using OVITO

- Choose (1) “Add modification” then (2) “Create isosurface” menu

The screenshot displays the OVITO software interface. The main 3D view shows a simulation cell with purple and green spheres. A red box highlights a specific region of the simulation cell. The left-side view shows a vertical slice of the simulation cell. The central menu is open, showing the 'Add modification...' option highlighted with a red box and the number '1'. The right-side panel shows the 'Add modification...' menu item highlighted with a red box and the number '2'. The bottom status bar shows '24 atoms' and '63 x 63 x 189 voxel grid'.

1

2

Particles Global Attr

24 atoms
63 x 63 x 189 voxel grid

Isosurface Rendering Using OVITO

- Adjust isolevel to draw a desired isosurface

The screenshot displays the OVITO Basic (Open Visualization Tool) interface. The main window is divided into four viewports: Top, Front, Left, and Perspective. The Top viewport shows a 3D representation of the simulation cell with particles and a green isosurface. The Front, Left, and Perspective views show different orientations of the same simulation cell. The right-hand panel contains the 'Create isosurface' and 'Isosurface' settings. The 'Create isosurface' panel shows the 'Isosurface' checkbox checked and the 'Isosurface' modification selected. The 'Isosurface' panel shows the 'Isosurface' settings, including the 'Isosurface' checkbox checked, the 'Surface color' set to a light blue color, and the 'Transparency' set to 0%. The 'Isosurface' panel also shows a histogram of the property field, with the 'Isosurface' panel highlighted by a red box.

OVITO Basic (Open Visualization Tool)

MoSe2-hole.cube [Cube]

Add modification...

Visual elements

- Simulation cell
- Particles
- Voxel grid
- Isosurface

Modifications

- Create isosurface

Data source

MoSe2-hole.cube [Cube]

Simulation cell

Particle types

Create isosurface

Operate on: Voxel grid: Voxel grid

Field quantity: Property

Isosurface: 0.0003

Histogram:

Count

Property

Field value range: [0, 0.0085018]

Isosurface

Surface

Surface color:

Transparency: 0%

- Smooth shading
- Flip surface orientation
- Highlight edges
- Cap polygons

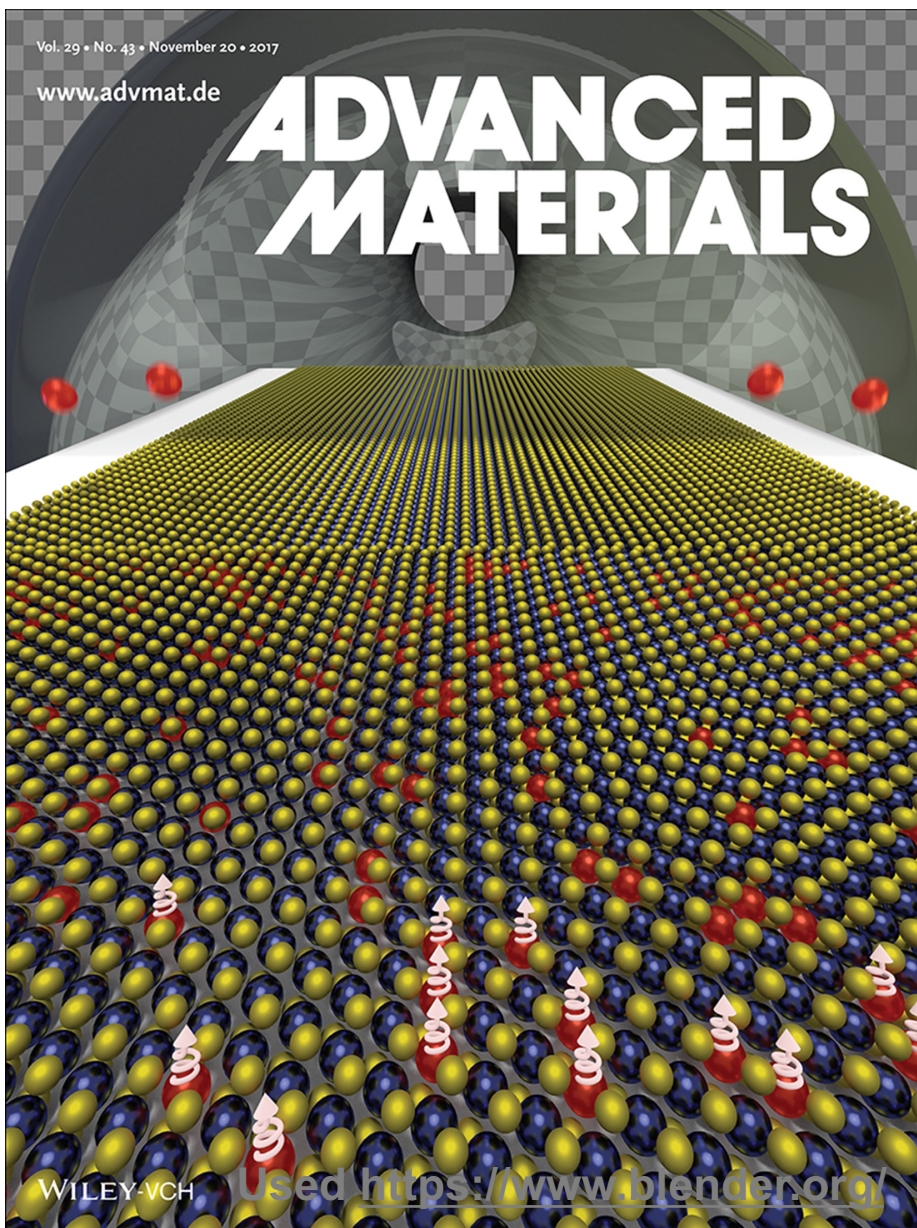
Cap color:

Transparency: 0%

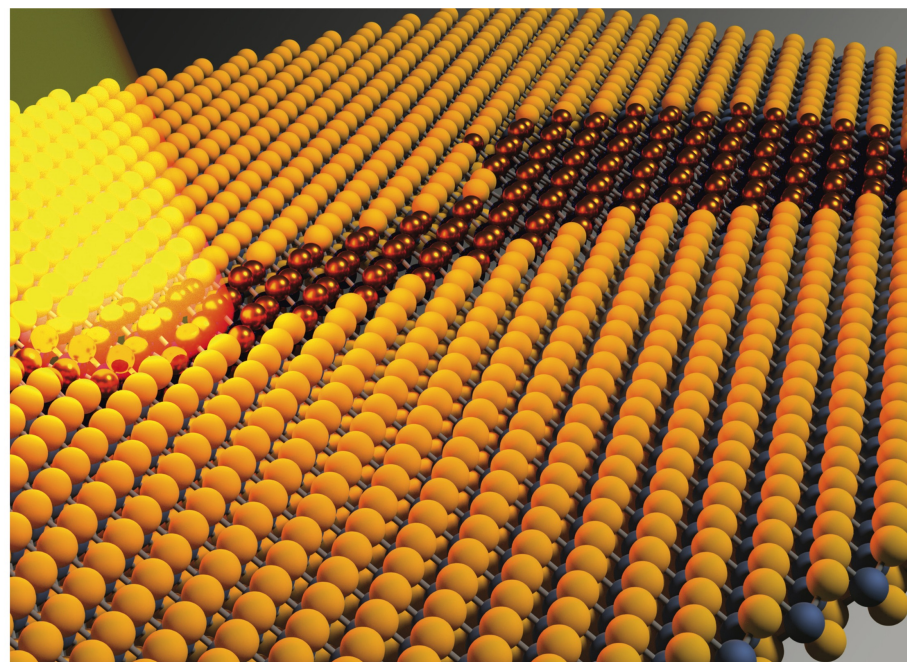
Particles Global Attributes Data Tables Voxel Grids Surfaces

Screenshot

Make Journal Covers



V. Kochat *et al.*, *Adv. Mater.* **29**, 1703754 ('17)

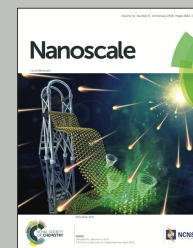


Showcasing research from Collaboratory for Advanced Computing and Simulations (CACS), University of Southern California, Los Angeles, USA.

Semiconductor–metal structural phase transformation in MoTe_2 monolayers by electronic excitation

Optical control of transformations between semiconducting and metallic phases of two-dimensional materials can open the door for phase patterning of heterostructures for 2D electronics and catalysis applications. This work shows how optically-induced changes to the electronic structure and Fermi surface of monolayer semiconductors couple to lattice distortions, resulting in a more facile phase transformation pathway. This work highlights photoexcitation as a viable technique for functionalizing these material systems.

As featured in:



See Aravind Krishnamoorthy *et al.*, *Nanoscale*, 2018, **10**, 2742.



rsc.li/nanoscale

Registered charity number: 207890

A. Krishnamoorthy *et al.*, *Nanoscale* **10**, 2742 ('18)

BES

Or report cover

BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

An Office of Science review sponsored jointly by
Advanced Scientific Computing Research and Basic Energy Sciences

16,661-atom QMD

Shimamura *et al.*,
Nano Lett.

14, 4090 ('14)

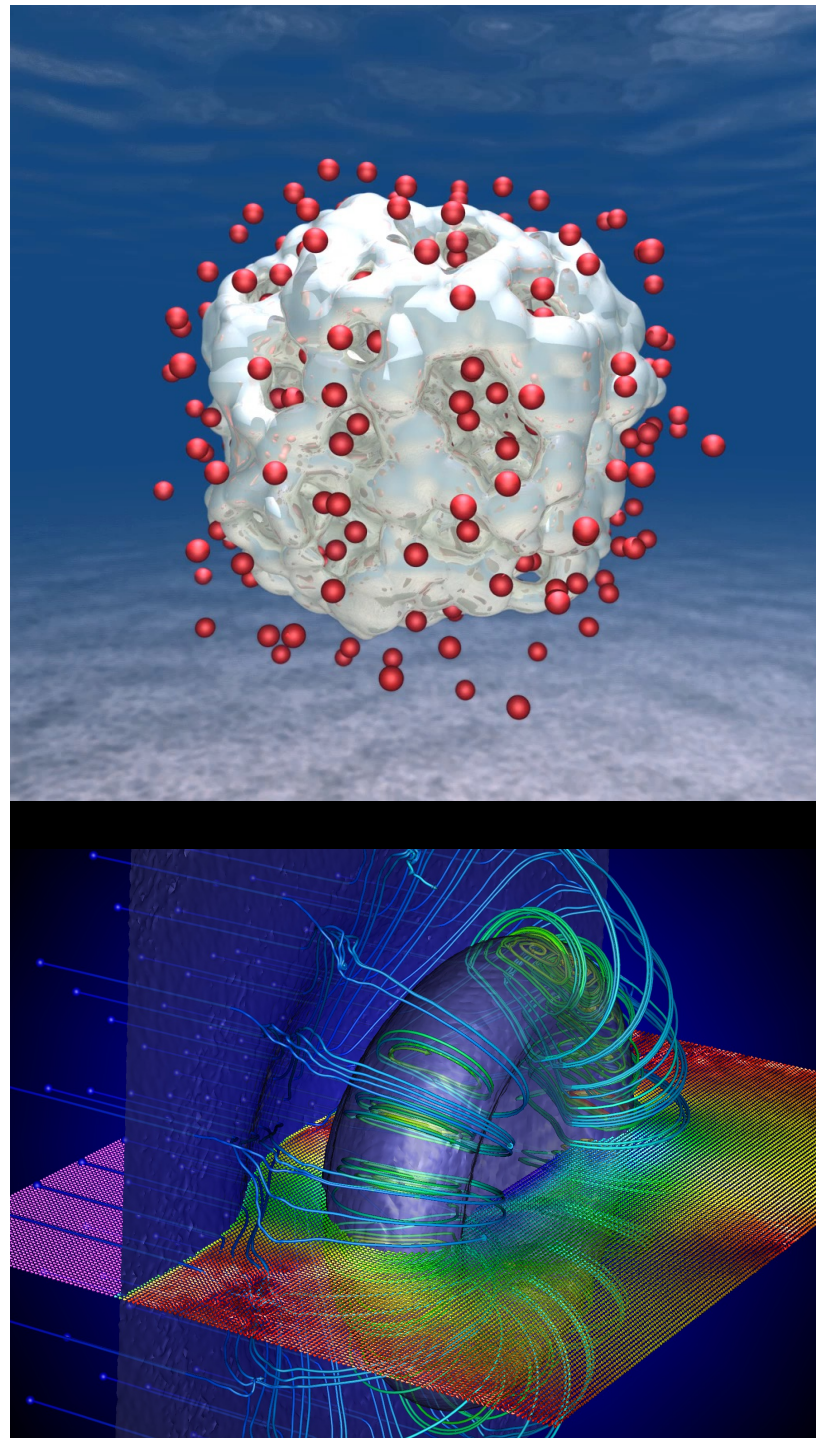
10⁹-atom RMD

Shekhar *et al.*,
Phys. Rev. Lett.

111, 184503 ('13)

NOVEMBER 3-5, 2015

ROCKVILLE, MARYLAND



Touch of Art



Where to Go from Here

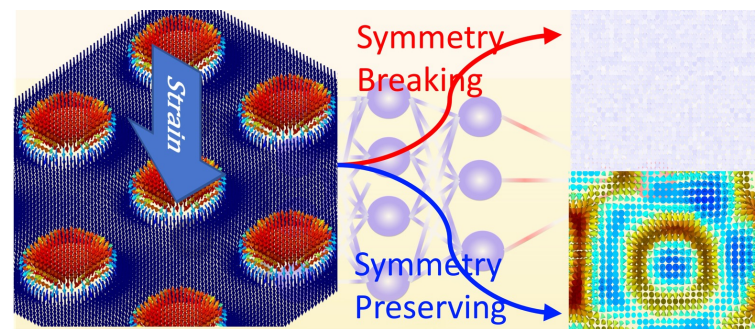
- Keep refining your visualization skill using the examples in this lecture as a starting point: “Seeing is believing”
- It’s the content that matters: “Summarize your work in 100 milliseconds or less... the importance of the table of contents image,” J. Buriak, *ACS Nano* 5, 7687 (’11); <https://aiichironakano.github.io/cs596/Buriak-ToC-ACSNano11.pdf>
- Appeal to fast thinking by ToC image, convince *via* slow thinking by abstract; see “Thinking about thinking” by Daniel Kahneman:
<https://www.edge.org/events/the-edge-master-class-2007-a-short-course-in-thinking-about-thinking>

Application of First-Principles-Based Artificial Neural Network Potentials to Multiscale-Shock Dynamics Simulations on Solid Materials

Masaaki Misawa,* Shogo Fukushima, Akihide Koura, Kohei Shimamura, Fuyuki Shimojo, Subodh Tiwari, Ken-ichi Nomura, Rajiv K. Kalia, Aiichiro Nakano, and Priya Vashishta

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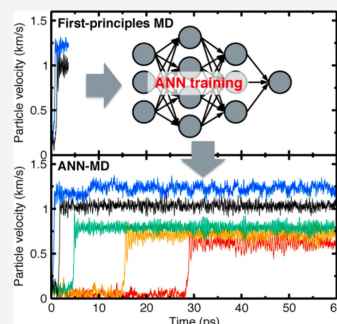
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ABSTRACT: The use of artificial neural network (ANN) potentials trained with first-principles calculations has emerged as a promising approach for molecular dynamics (MD) simulations encompassing large space and time scales while retaining first-principles accuracy. To date, however, the application of ANN-MD has been limited to *near-equilibrium* processes. Here we combine first-principles-trained ANN-MD with multiscale shock theory (MSST) to successfully describe *far-from-equilibrium* shock phenomena. Our ANN-MSST-MD approach describes shock-wave propagation in solids with first-principles accuracy but a 5000 times shorter computing time. Accordingly, ANN-MD-MSST was able to resolve fine, long-time elastic deformation at low shock speed, which was impossible with first-principles MD because of the high computational cost. This work thus lays a foundation of ANN-MD simulation to study a wide range of far-from-equilibrium processes.



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