VMD & OVITO Visualization of Molecular Dynamics

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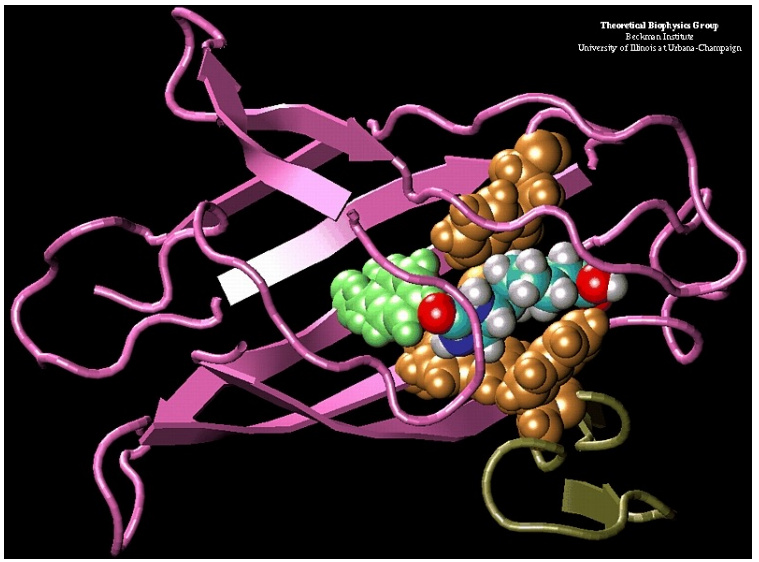
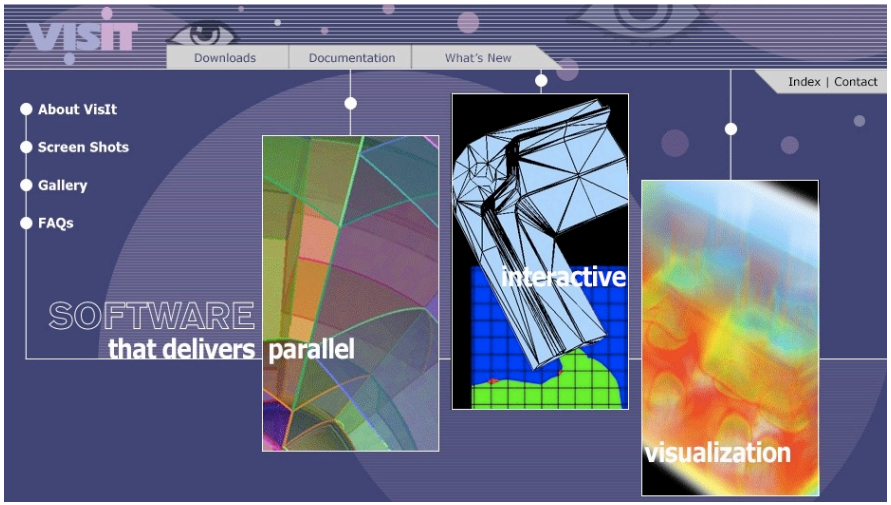
Goal: Publication-quality image of "your" data
(gallery as final project?)

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

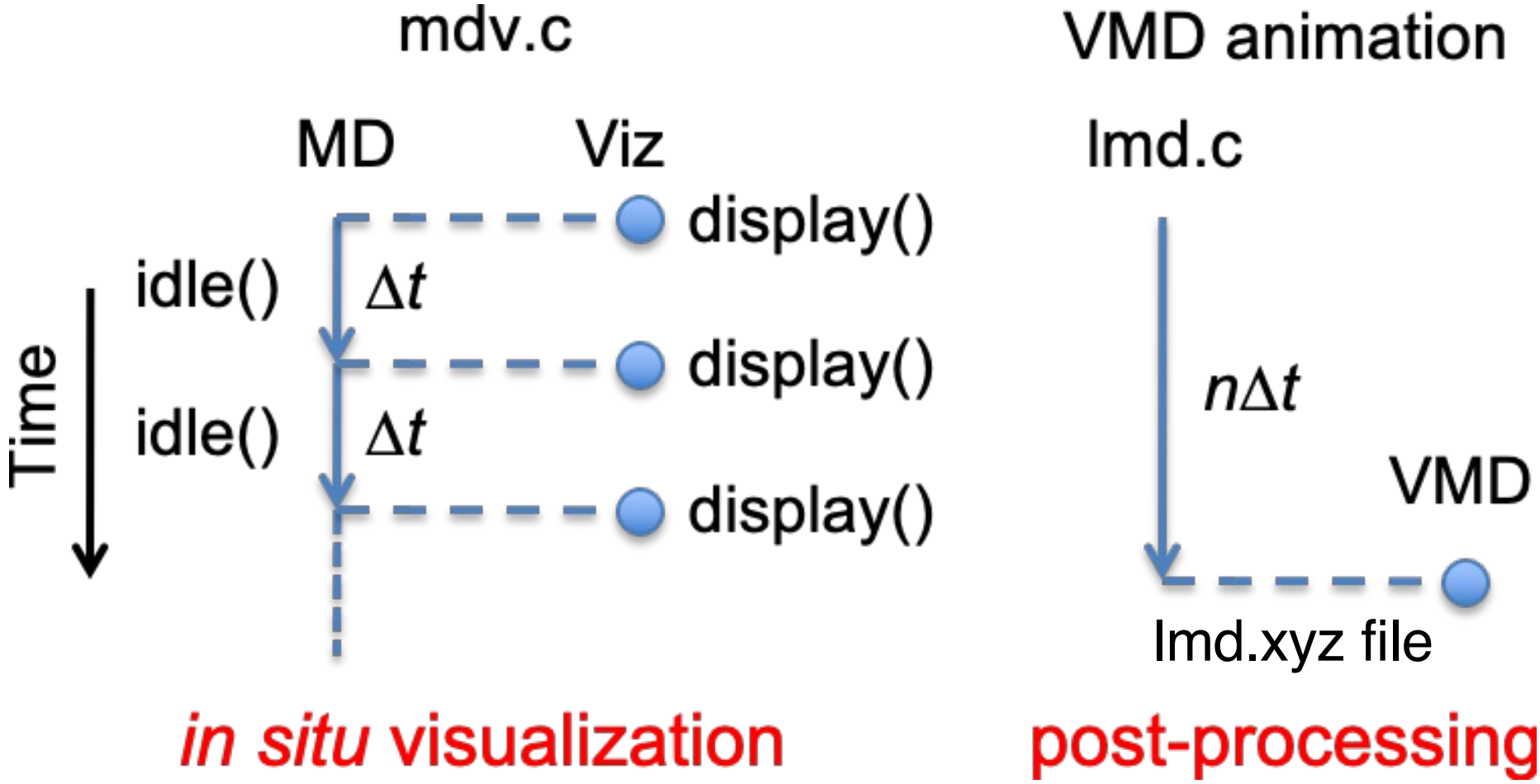
Scientific Visualization Tools

- **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



Visual debugging & control

***In situ* visualization using common visualization software?**

See B. Whitlock *et al.*, *PGV11*

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 (2022-04-27) Platforms:

Latest pre-release ALPHA test version

- **Source Code**
- **LINUX_64 (RHEL 7+) OpenGL, CUDA, OptiX RTX, OSPRay** (Linux (RHEL 7+) 64-bit Intel/AMD x86_64 SSE/AVX+ with CUDA 10, OptiX6.5 RTX, OSPRay)
- **LINUX_64 (RHEL 7+) OpenGL, CUDA, OptiX RTX, OSPRay, RTX RTRT** (Linux (RHEL 7+) 64-bit Intel/AMD x86_64 SSE/AVX+ with CUDA 10, OptiX6.5 RTX, OSPRay, RTX RTRT)
- **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)
- **Windows 64-bit, CUDA, OptiX, OSPRay (64-bit Intel x86_64)** (Windows 10)

Version 1.9.3 (2016-11-30) Platforms:

We recommend that all users upgrade to VMD 1.9.3

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`

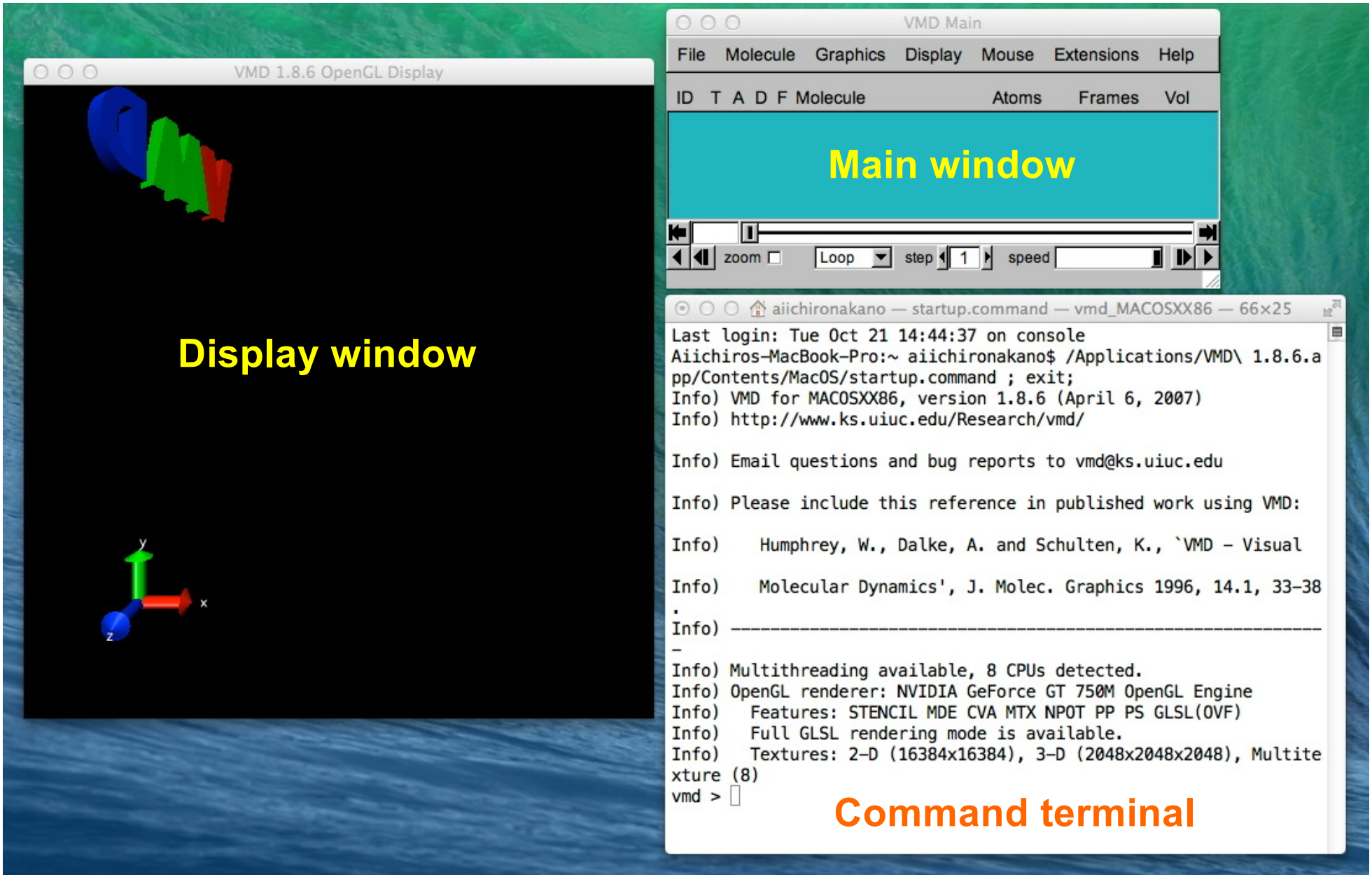
```
#define SIGMA 3.4 // Lennard-Jones length scale in angstrom
FILE *fxyz;
...
int main(int argc, char **argv) () {
  ...
  fxyz = fopen("lmd.xyz","w");
  ... // Main MD for loop
  fclose(fxyz);
  ...
}
...
void EvalProps() {
  ...
  fprintf(fxyz,"%d\n",nAtom);
  fprintf(fxyz,"Molecular dynamics simulation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

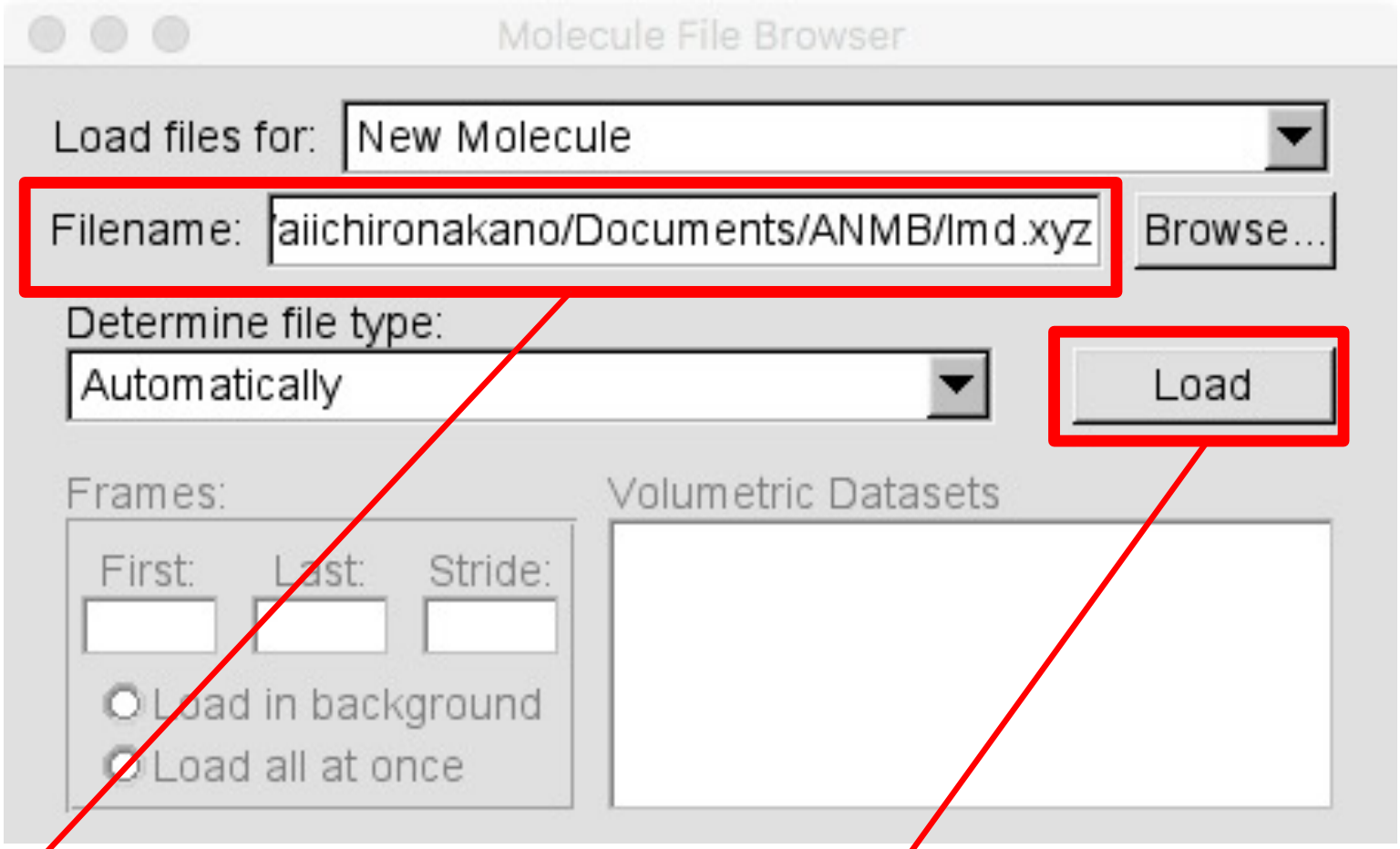
Start VMD

- It will open 3 windows



Load the MD-Trajectory XYZ File

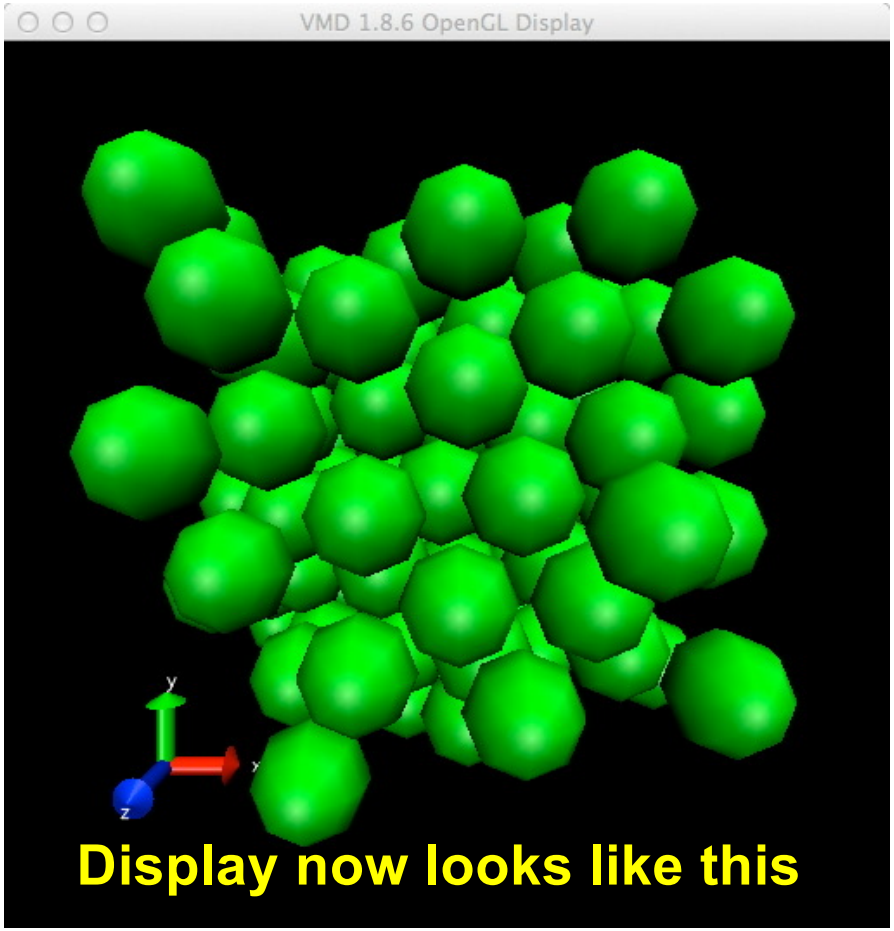
- **In the File menu in the VMD main window, select New Molecule; the following new window will open.**

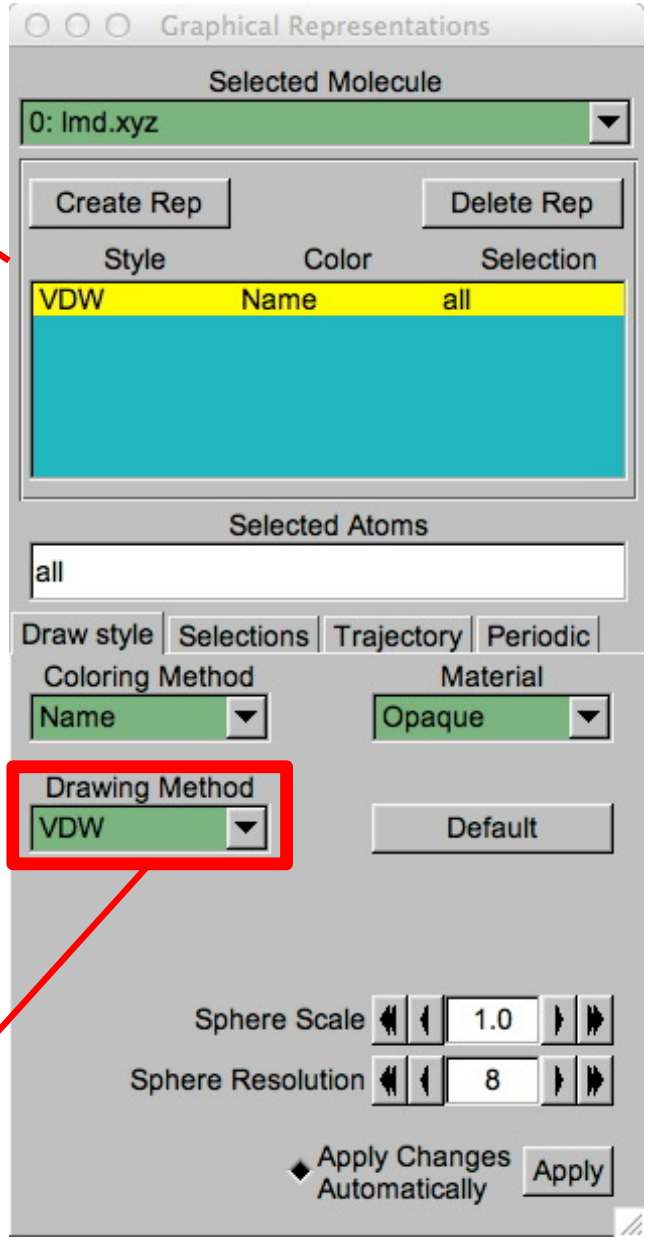


- **Drag and drop the XYZ file you have created in the Filename field (or press the browse button to locate the file).**
- **Click the Load button to load the file.**

Choose the Graphic Representation

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

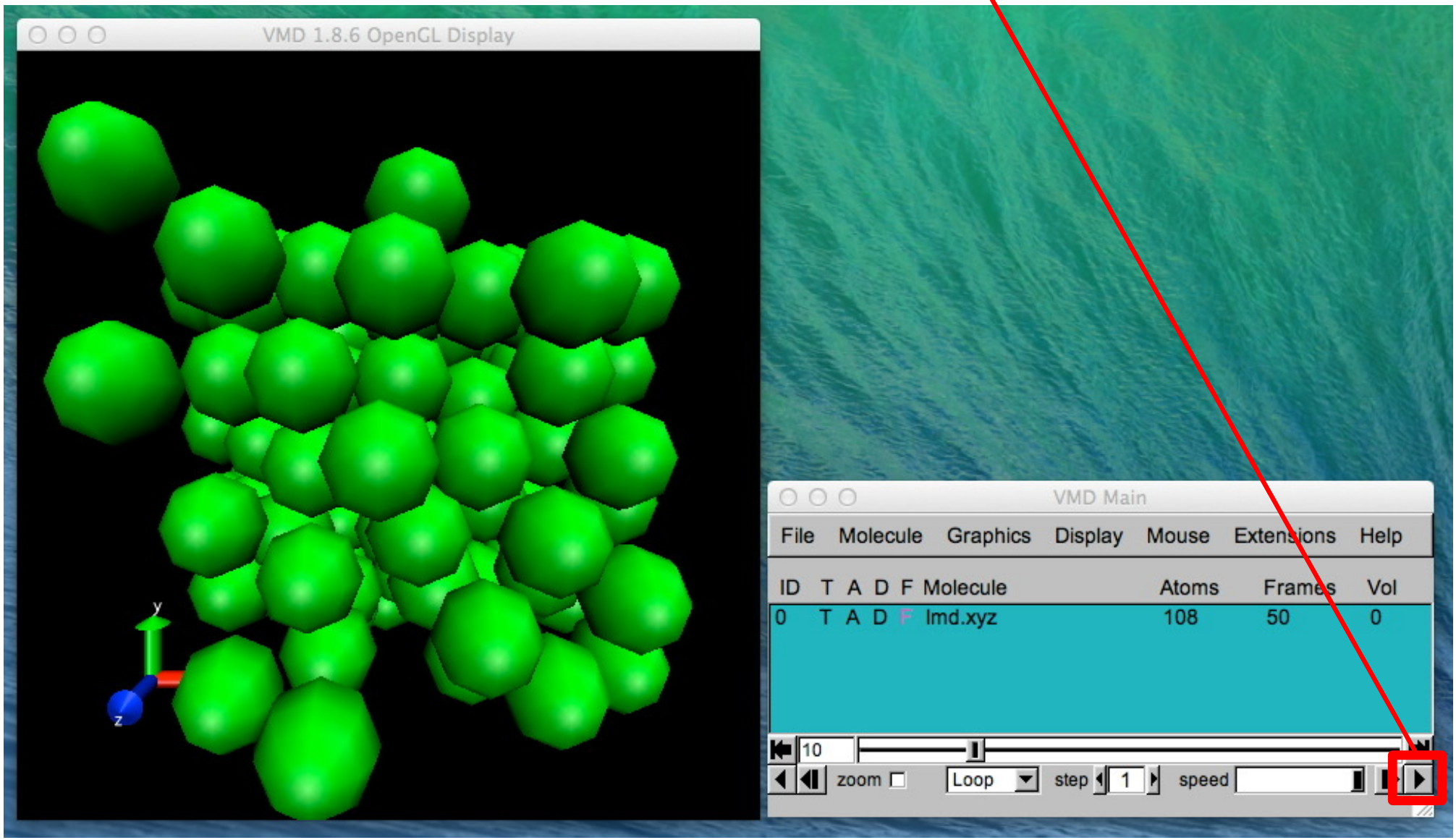




- **In the Drawing Method menu, choose the VDW (van der Waals radius) representation.**

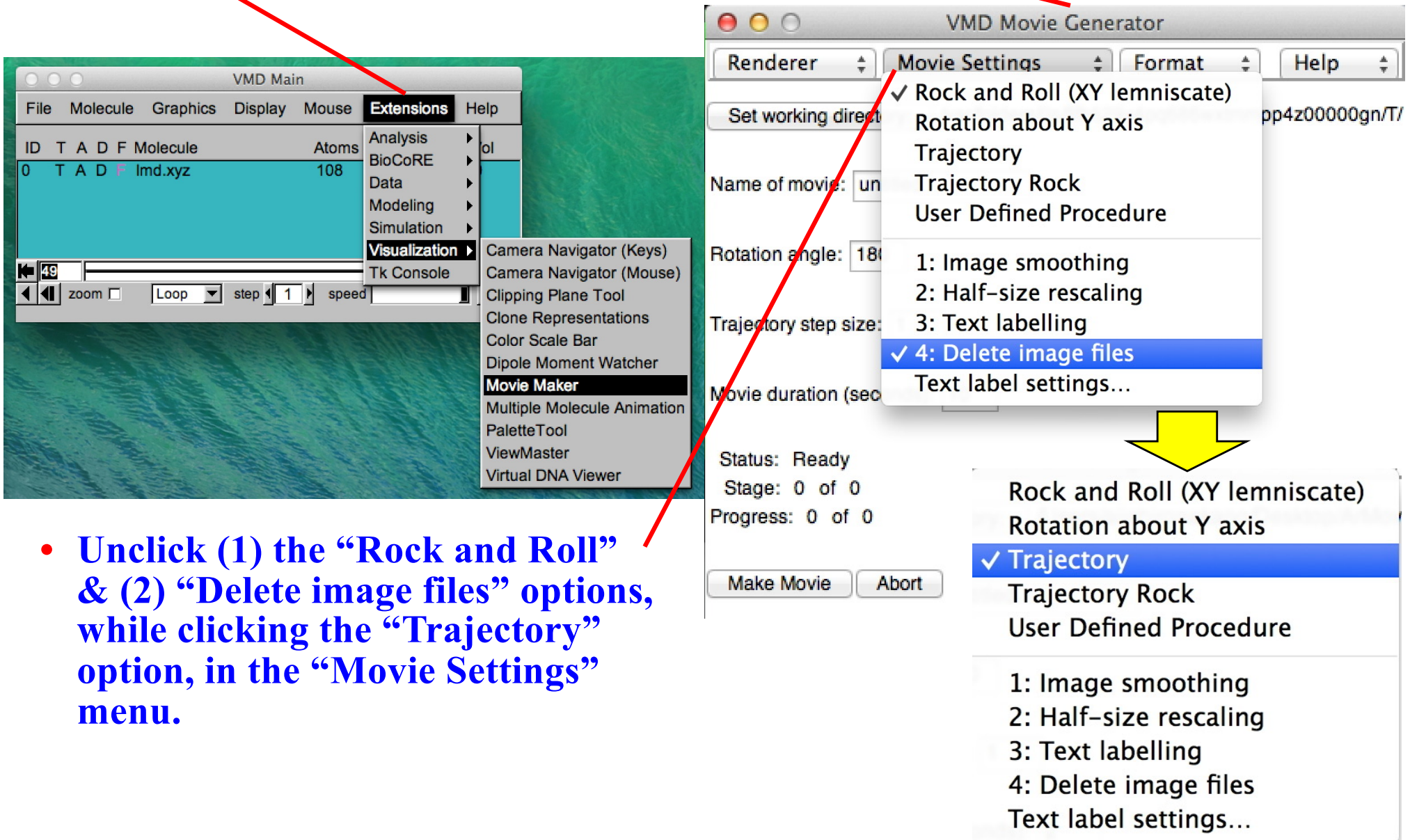
Animation

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



Optional: Creating a Movie File (1)

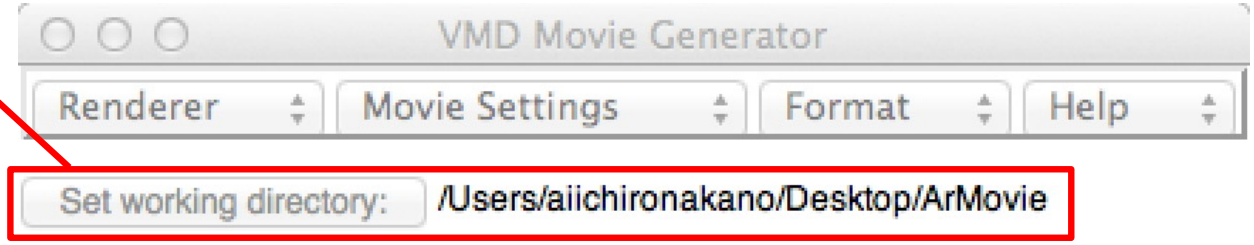
- **Choose the Extensions → Visualization → Movie Maker menu; this will open a VMD Movie Generator window.**

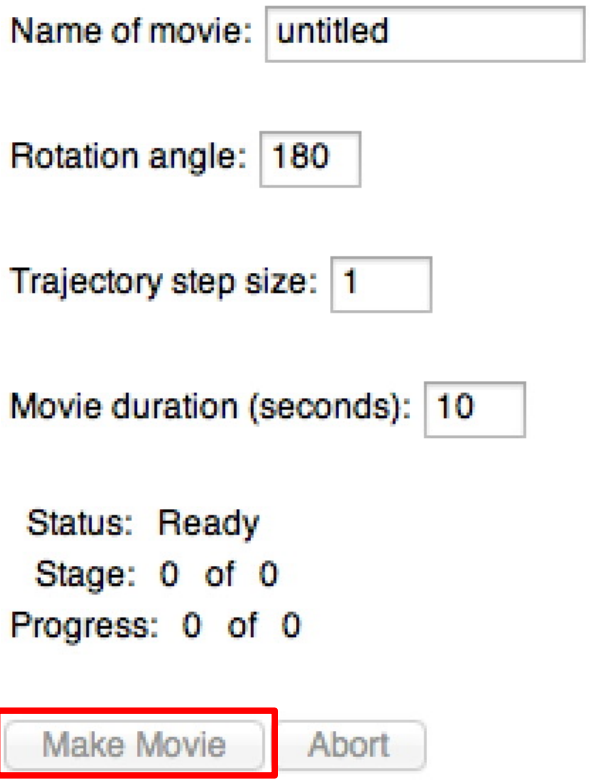


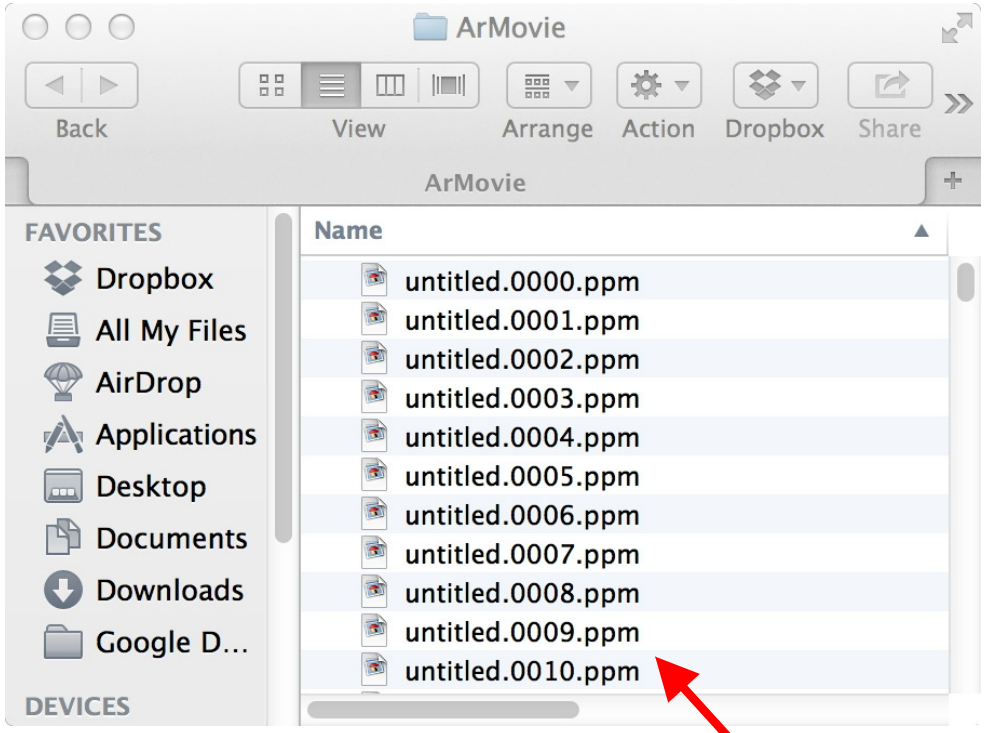
- **Unclick (1) the "Rock and Roll" & (2) "Delete image files" options, while clicking the "Trajectory" option, in the "Movie Settings" menu.**

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.**



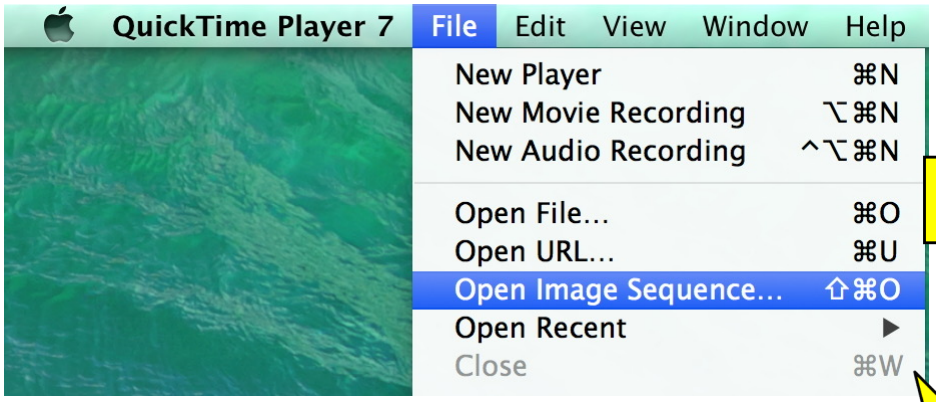


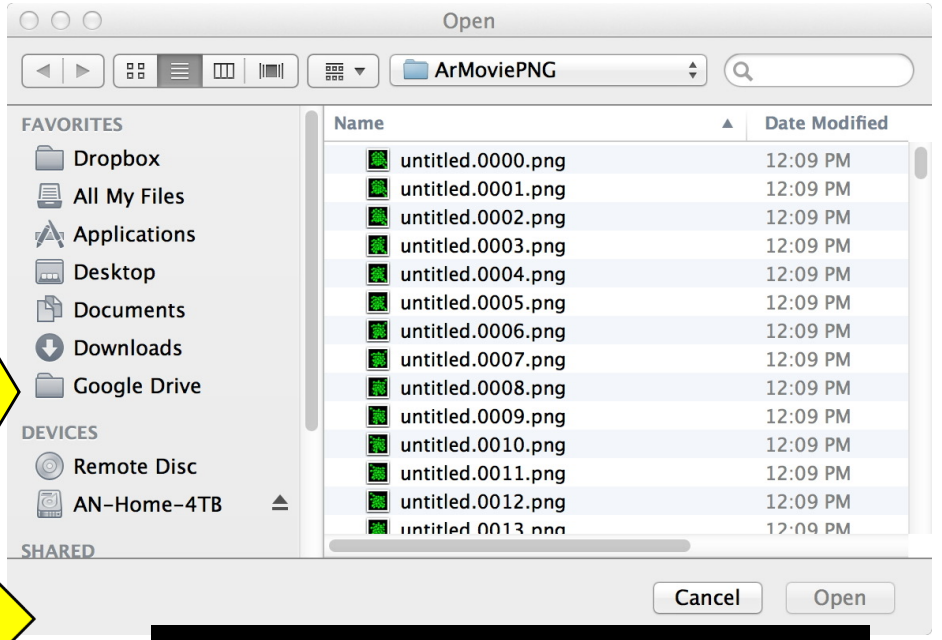


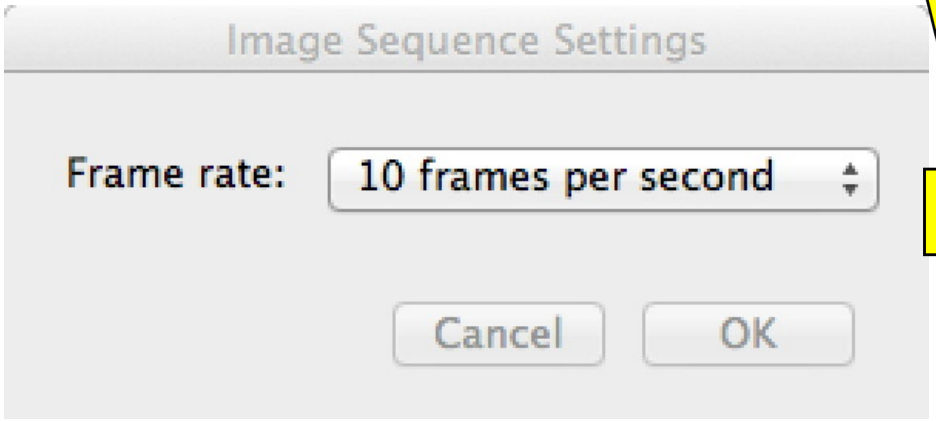
- **Click the "Make Movie" button; you will find image files in the directory.**

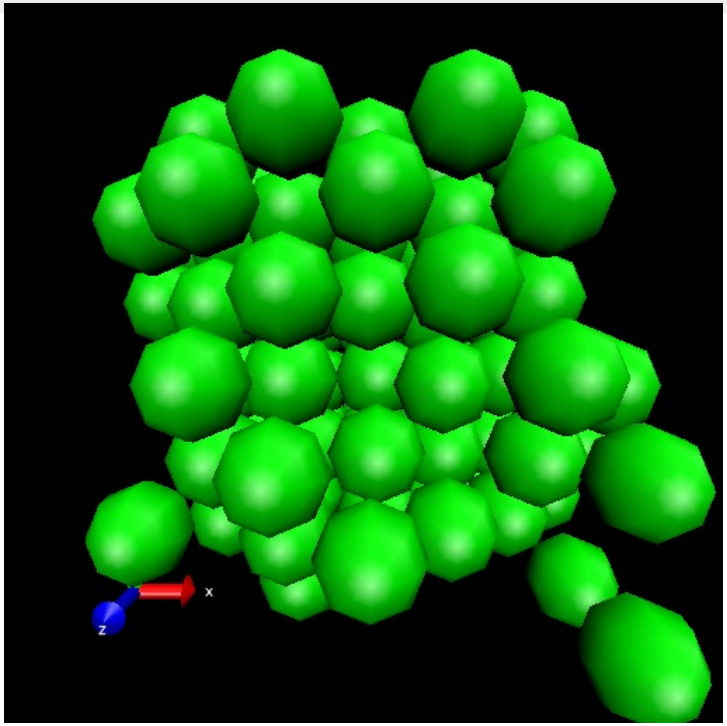
Optional: Creating a Movie File (3)

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







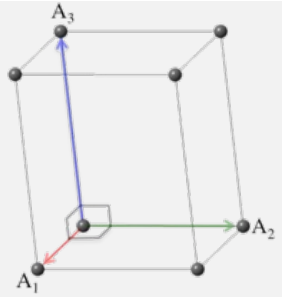


- Before this step, we have converted the PPM (portable pixmap) image files created by VMD to PNG (portable network graphics) image files that QuickTime Player can read, using the GraphicsConverter software.

Gaussian Cube File Format

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

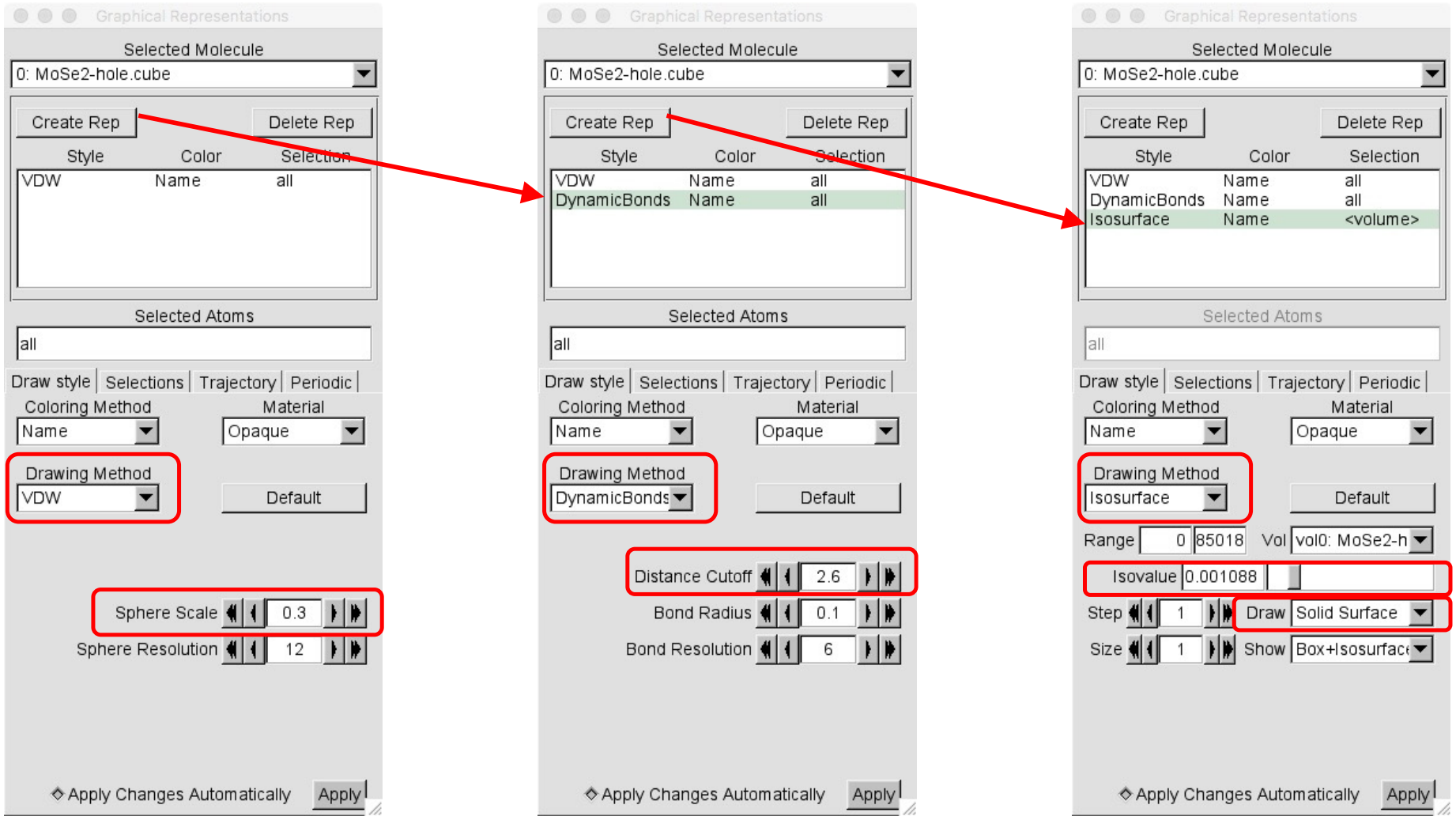
```
<header>
<comment>
 24    0.000000    0.000000    0.000000  // # atoms & origin
 63    0.198958    0.000000    0.000000  // # of voxels 1st axis
 63   -0.099479    0.172302    0.000000  //              2nd
189    0.000000    0.000000    0.194054  //              3rd
 42    0.000000   -0.000013    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)
```



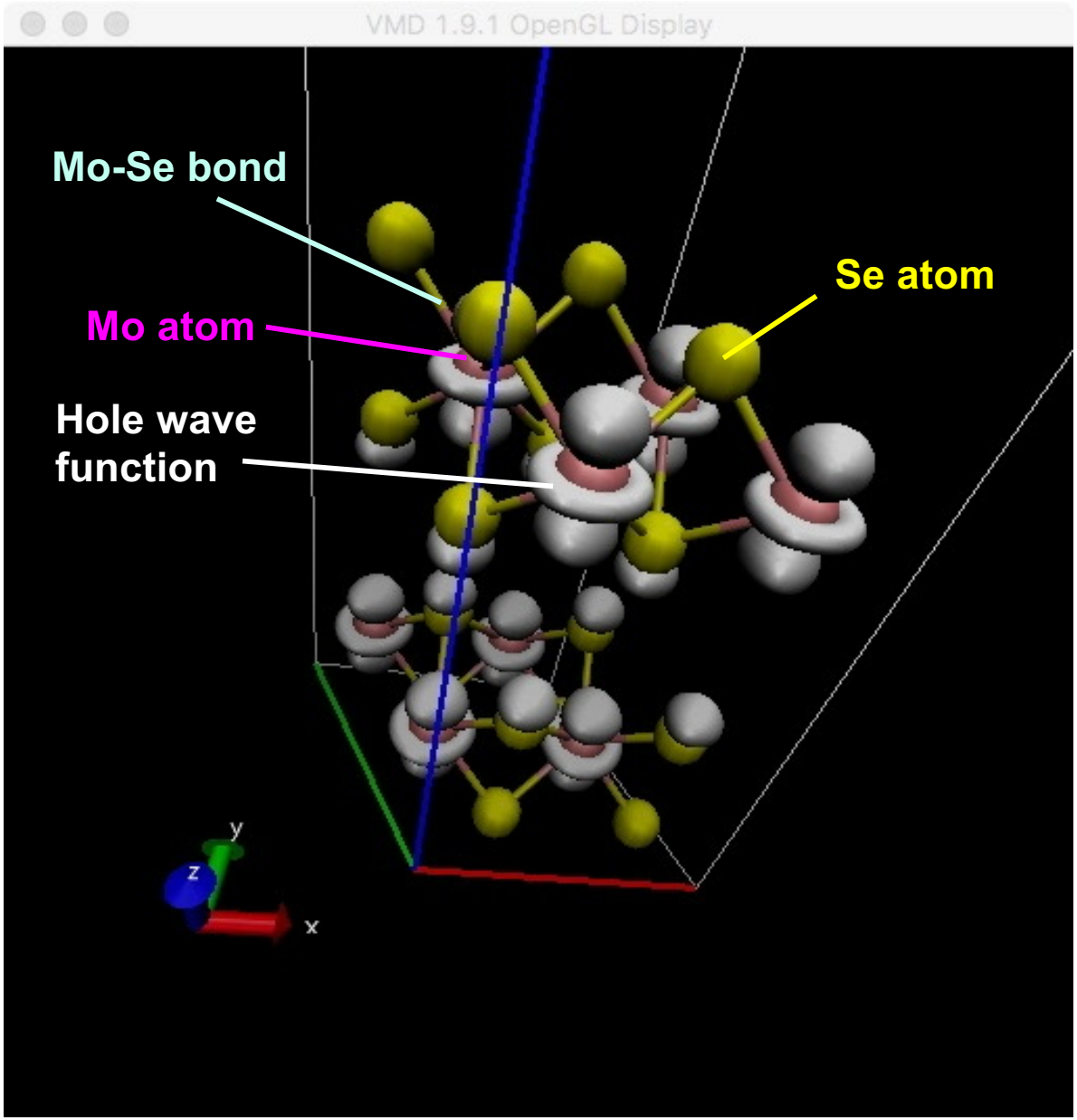

```
for (ix=0;ix<NX;ix++) {
  for (iy=0;iy<NY;iy++) {
    for (iz=0;iz<NZ;iz++) {
      printf("%g ",data[ix][iy][iz]); if (iz % 6 == 5) printf("\n");
    } printf("\n");
  }
}
```

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)

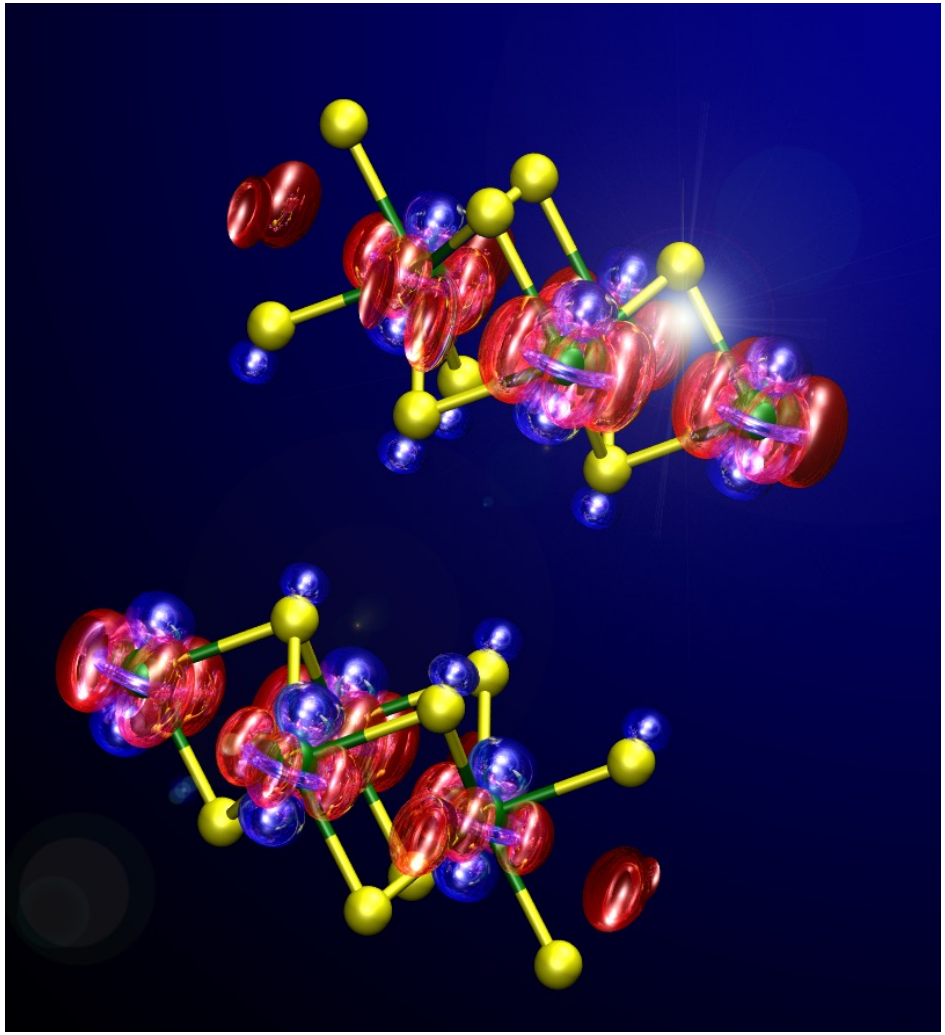


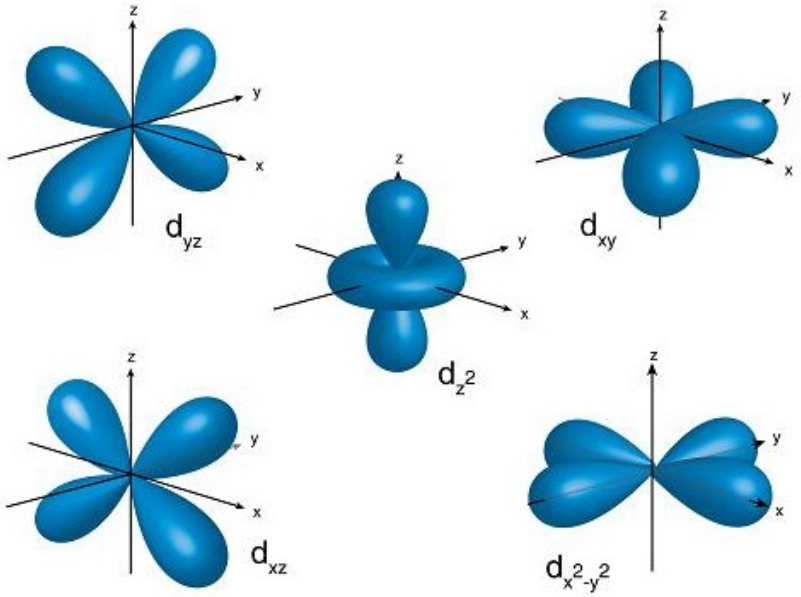
Isosurface Rendering



Wave Functions in $MoSe_2$ Bilayer

- Highest occupied states (blue) are d_{z2}-like
- Lowest unoccupied states (red) are d_{xy}-like



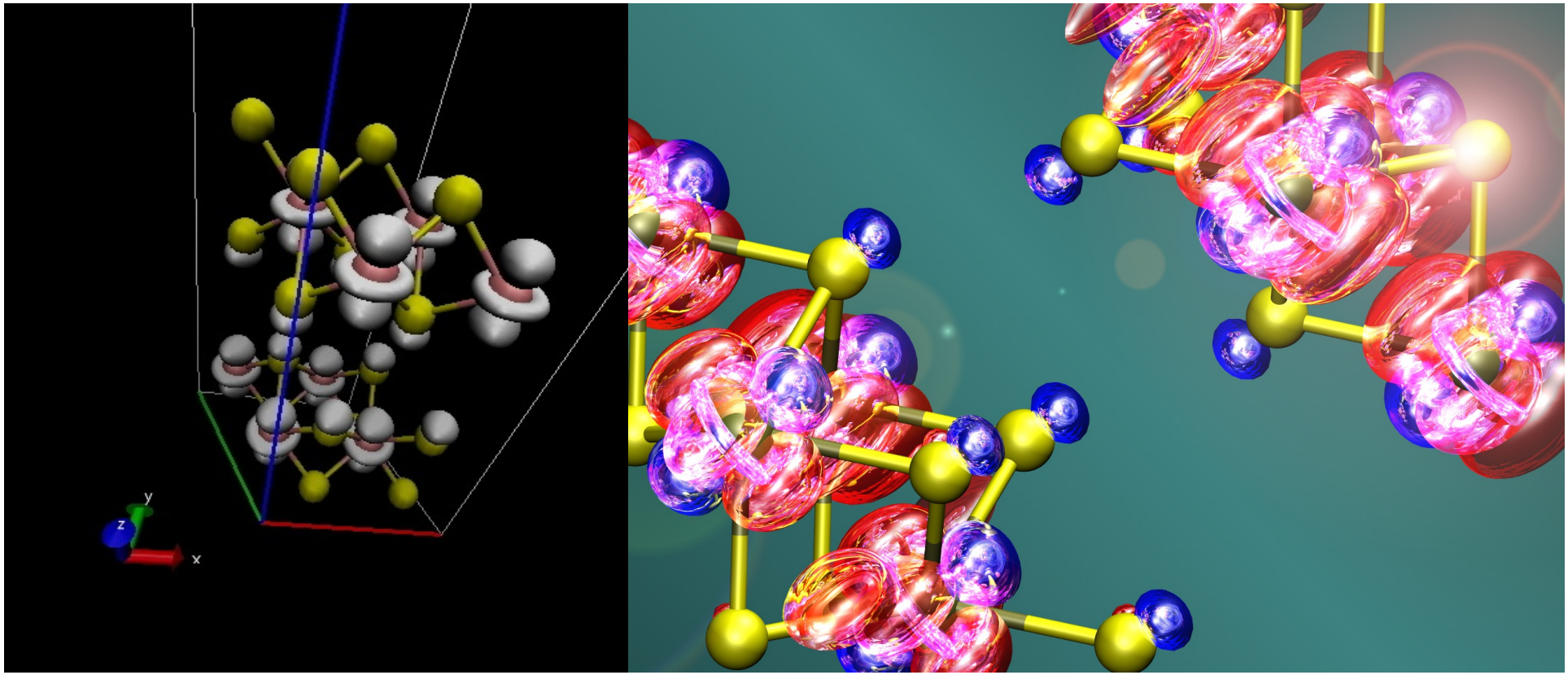


Electron
Hole

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

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

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

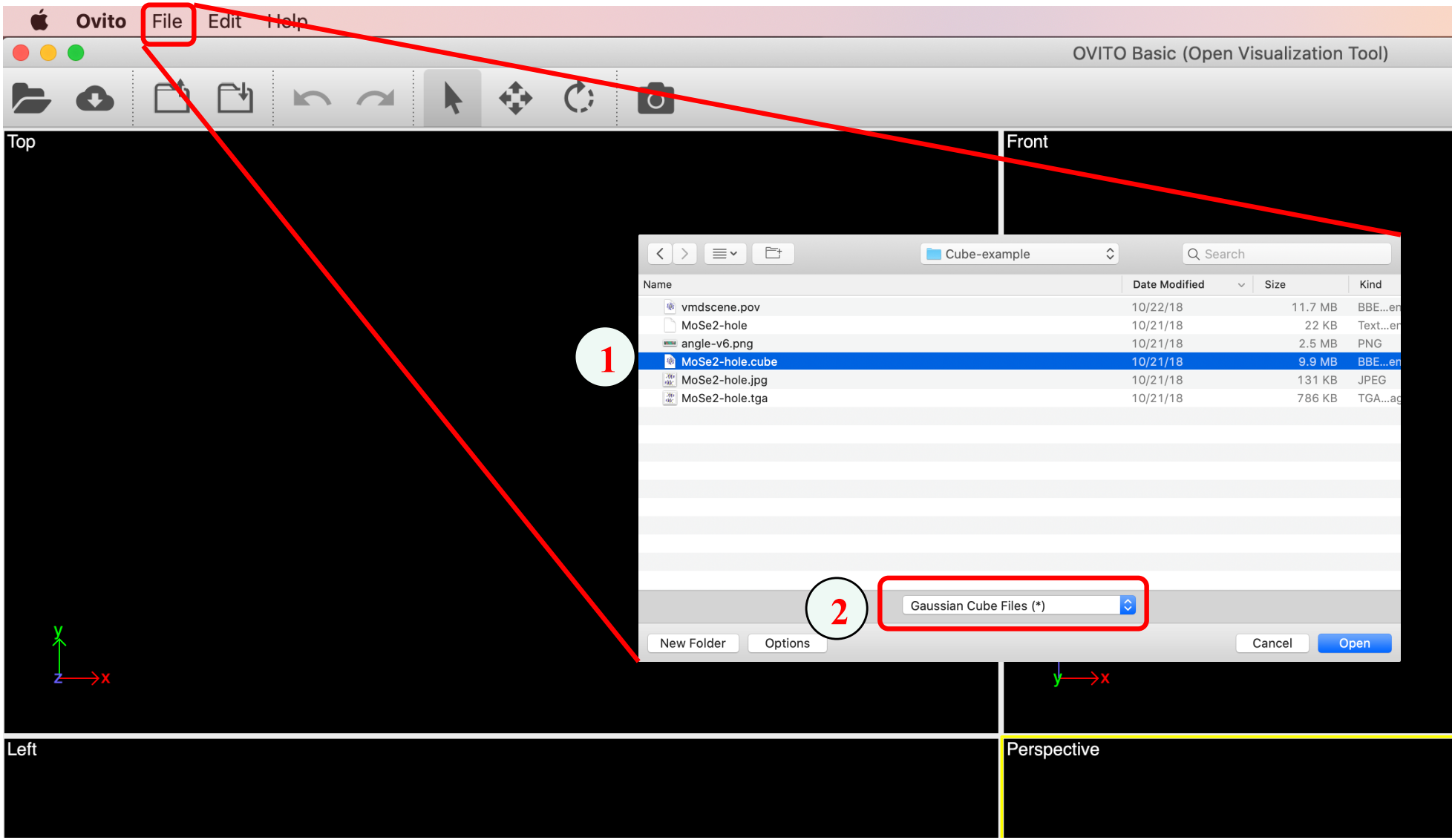
Professional version — full functionality

Version 3.9.2 — 31 Aug, 2023

Unfortunately, the isosurface feature is no longer free!

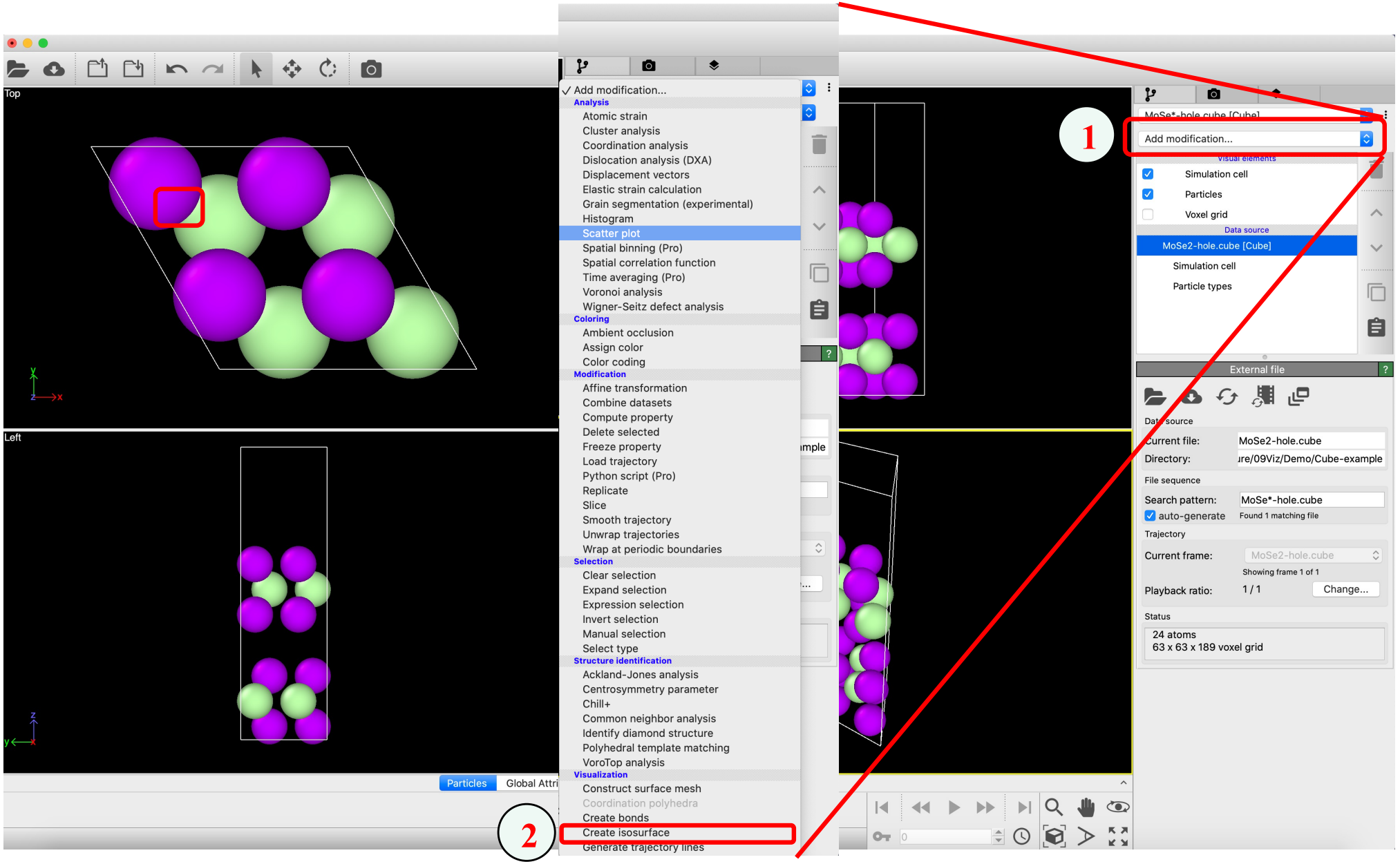
Isosurface Rendering Using OVITO

- 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



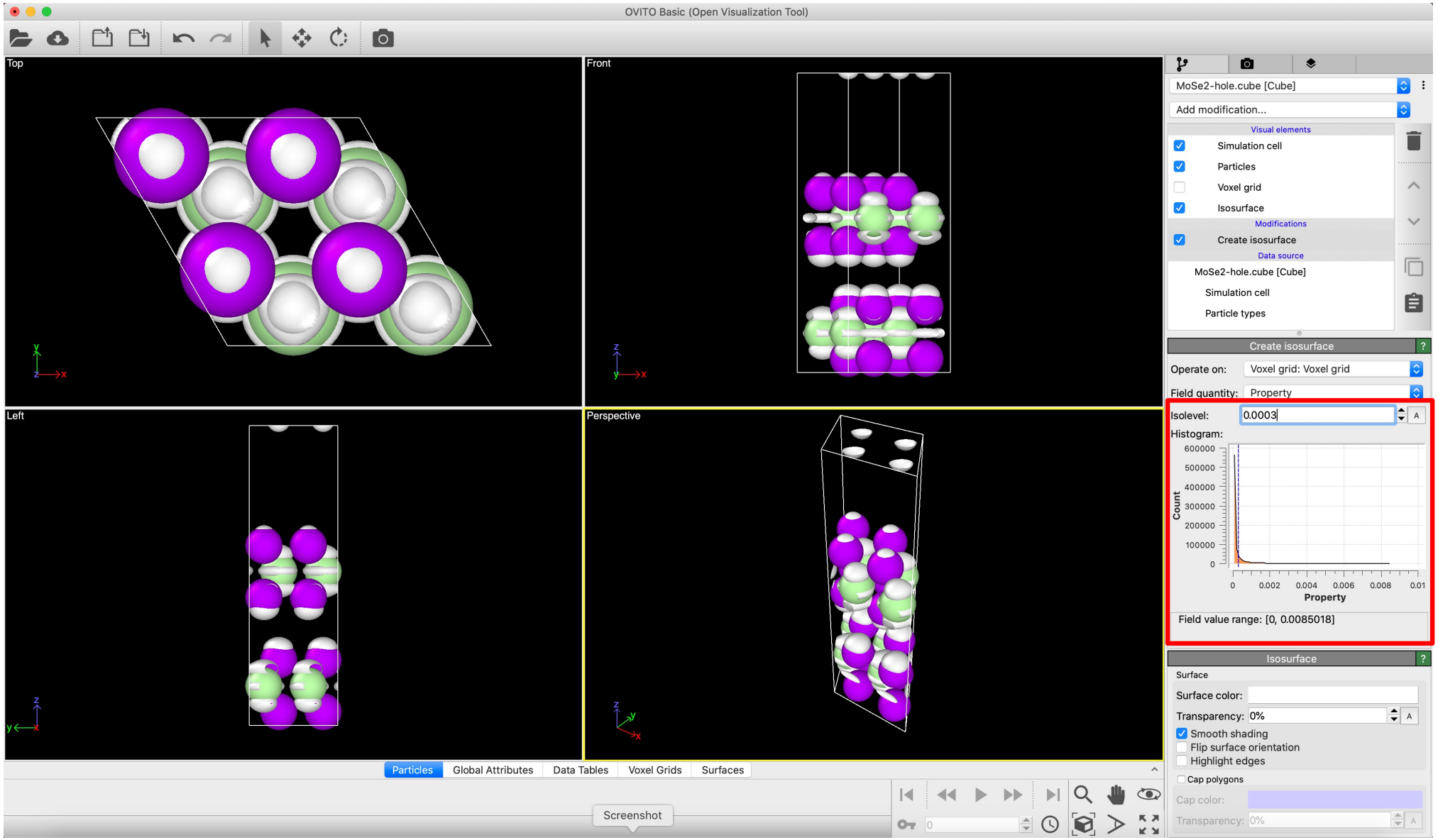
Isosurface Rendering Using OVITO

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



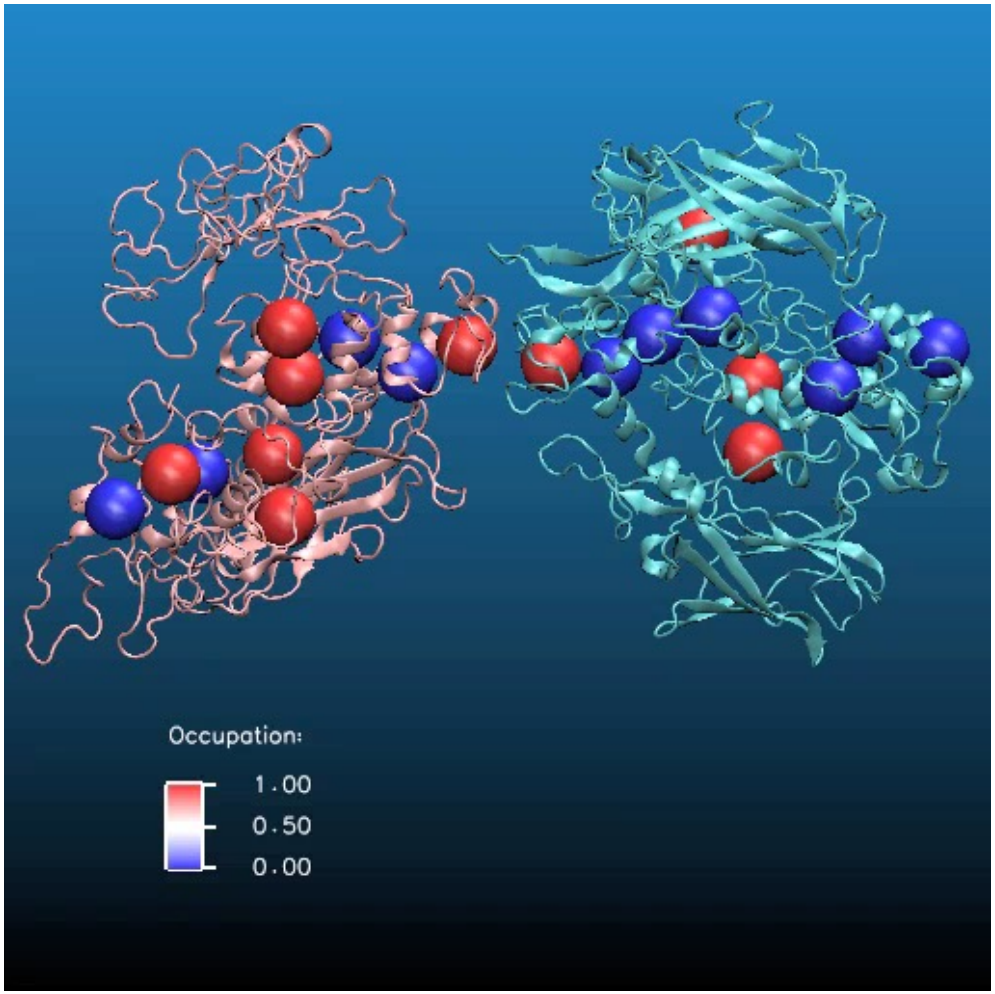
Isosurface Rendering Using OVITO

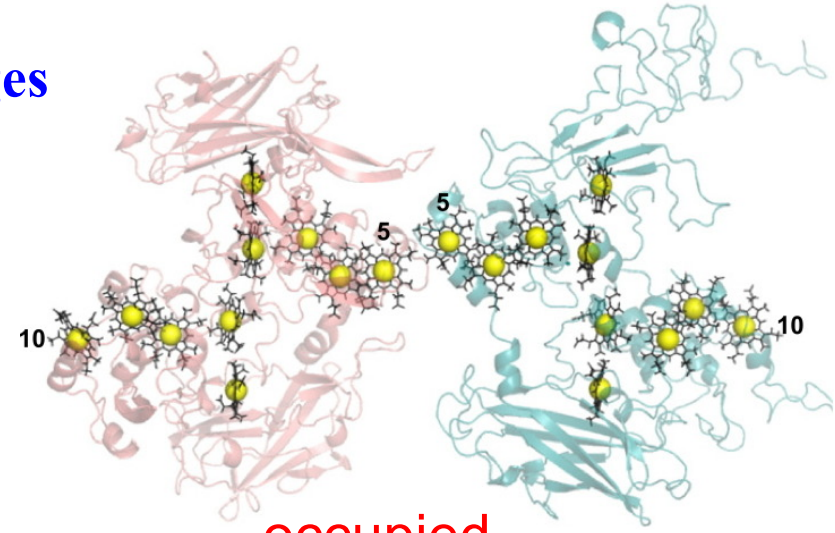
- **Adjust isolevel to draw a desired isosurface**



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**





occupied

Fe^{2+}

oxidation

reduction

e^- e^-

Fe^{3+}

unoccupied

C. M. Nakano, H.S. Byun, H. Ma, T. Wei, & M.Y. El-Naggar, *Comput. Phys. Commun.* **193**, 1 ('15)

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
%source userb.tcl
```

  Absolute path that contains Tcl script named 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**

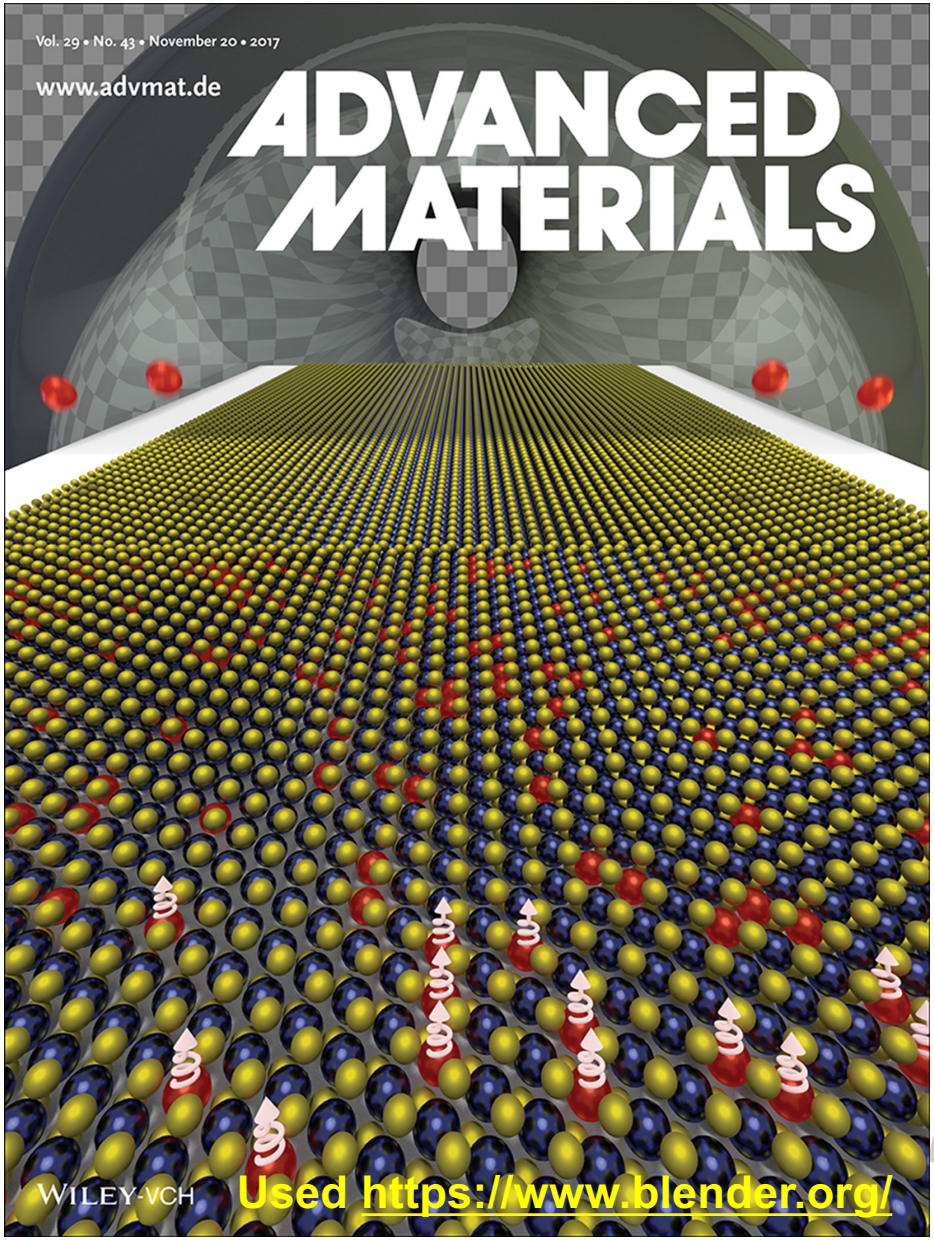
https://aiichironakano.github.io/cs596/src/viz/userb.tcl

```
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]]
      }
  }
}
```

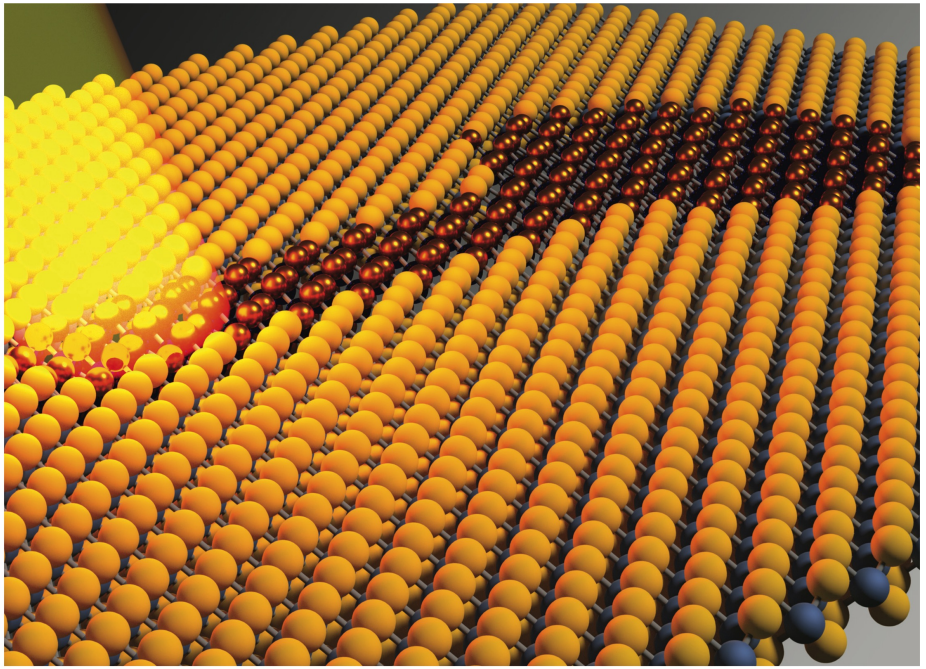
Find more examples: https://www.ks.uiuc.edu/Research/vmd/script_library/

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

Make Journal Covers



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

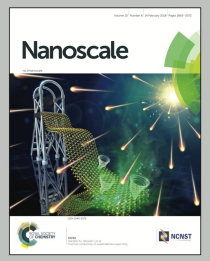


Showcasing research from Collaboratory for Advanced Computing and Simulations (CACS), University of Southern California, Los Angeles, USA.

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.

ROYAL SOCIETY OF CHEMISTRY

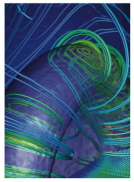
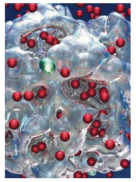
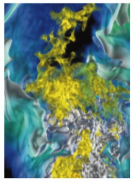
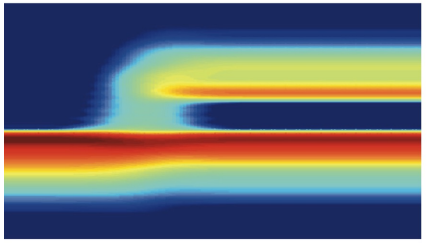
rsc.li/nanoscale

Registered charity number: 207890

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

Or report cover

BES

BASIC ENERGY SCIENCES

EXASCALE REQUIREMENTS REVIEW

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

NOVEMBER 3–5, 2015

ROCKVILLE, MARYLAND

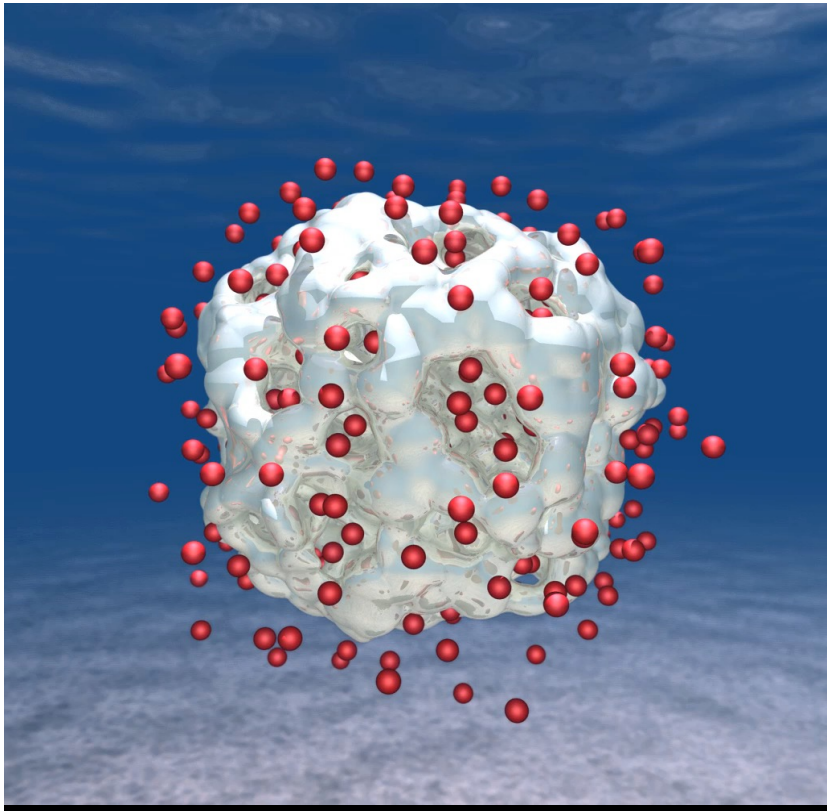
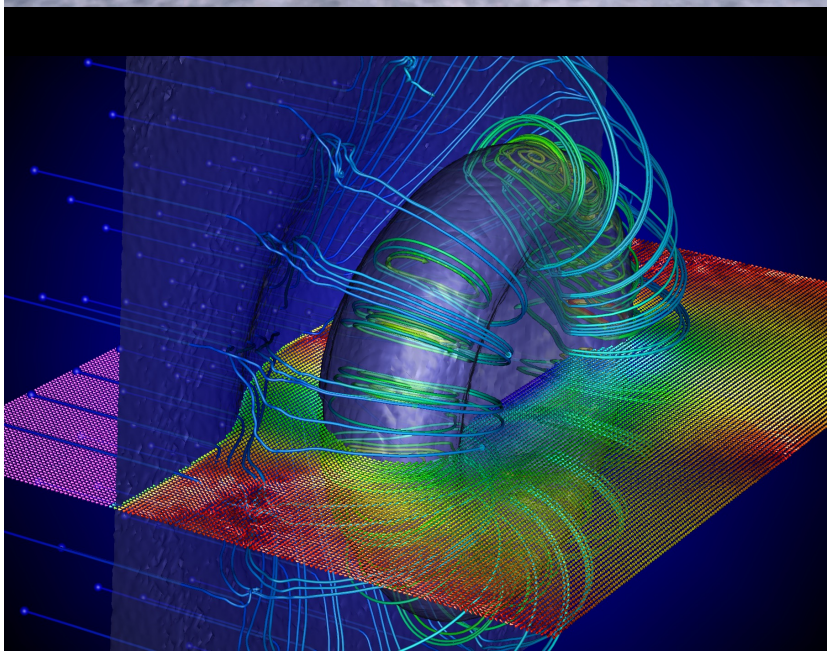
16,661-atom QMD

Shimamura *et al.*,
Nano Lett.
14, 4090 ('14)

10^9-atom RMD

Shekhar *et al.*,
Phys. Rev. Lett.
111, 184503 ('13)

U.S. DEPARTMENT OF ENERGY

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A. Nazarova *et al.*, *JCIM* **61**, 2175 ('21)

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

Cite This: *J. Phys. Chem. Lett.* 2020, 11, 4536–4541 | Read Online

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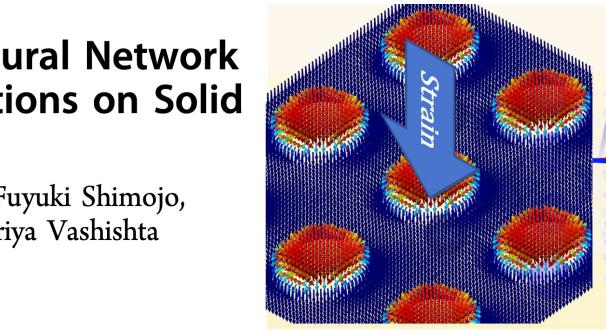
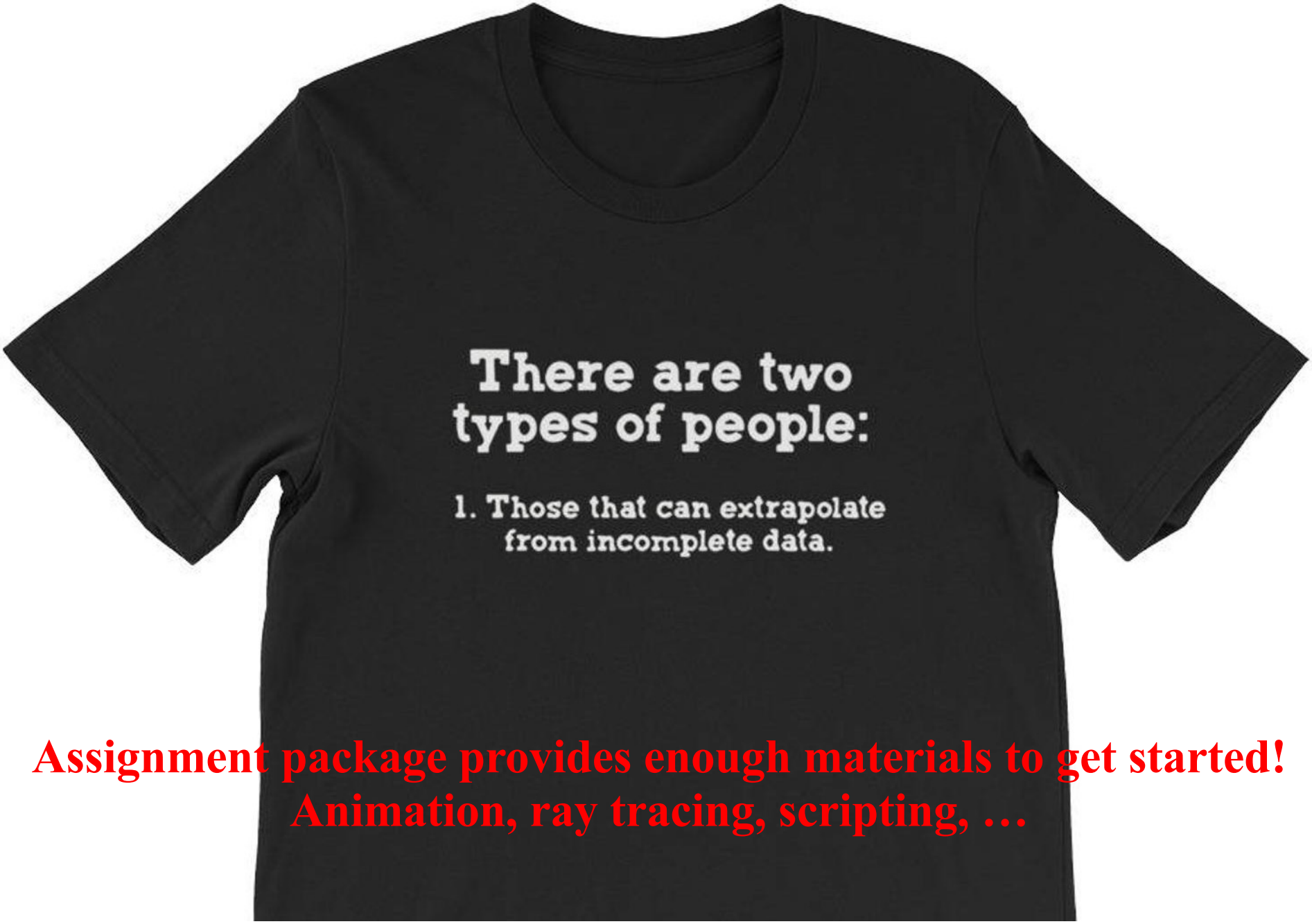
ABSTRACT: The use of artificial neural network (ANN) potentials trained with first-principles calculations has emerged as a promising approach for molecular dynamics (MD) simulations encompassing large space and time scales while retaining first-principles accuracy. To date, however, the application 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.



Squishing skyrmions: symmetry-guided dynamic transformation of polar topologies under compression

T. Linker *et al.*, *J. Phys. Chem. Lett.* **13**, 11335 ('22)

Where to Go from Here



Assignment package provides enough materials to get started!

Animation, ray tracing, scripting, …