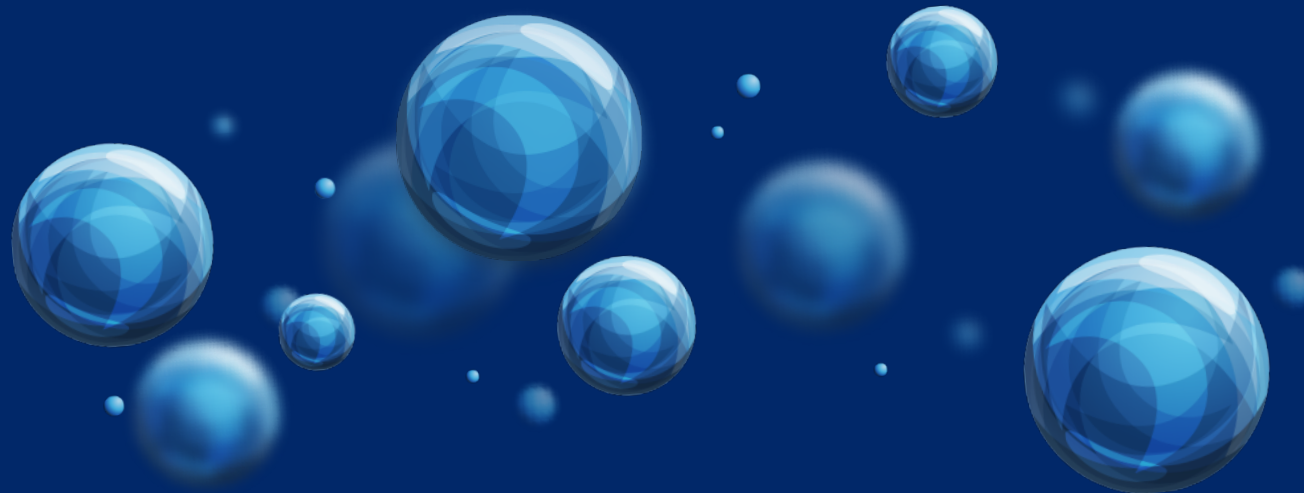


Which Visualizer is Suitable for Your Research?

Speaker : Kyungyeol Gu

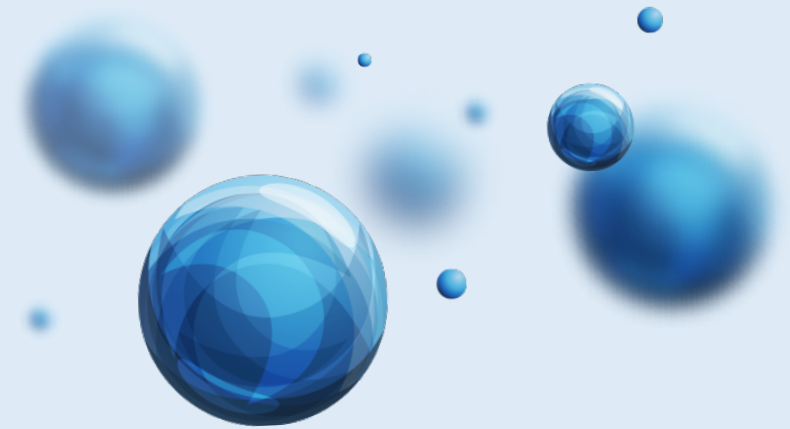
Virtual Lab. Inc.



Which Visualizer is Suitable for Your Research?

0 About us

About us



ABOUT US

Introduction

Members

We started this business to break barriers and help everyone do their own simulation in easy-to-learn and user-friendly web environment. Our proprietary web-based simulation service 'Materials Square', designed with an intuitive interface to the computing environment of the cloud server, provides a 'comprehensive integrated simulation environment offering service' that only pays for services of using.

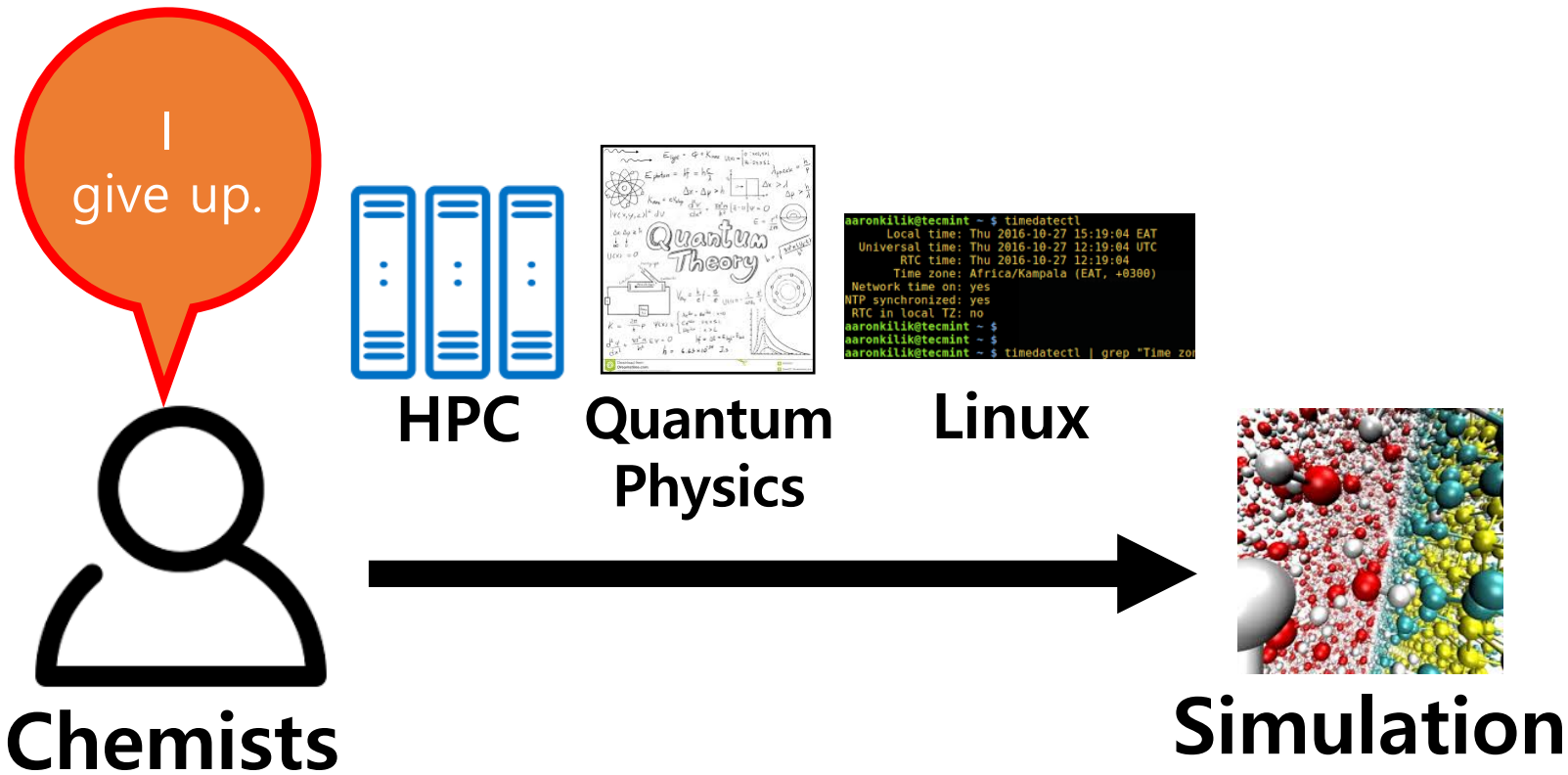
Legal Name Virtual Lab. Inc.

Founded Date 2016/01/28

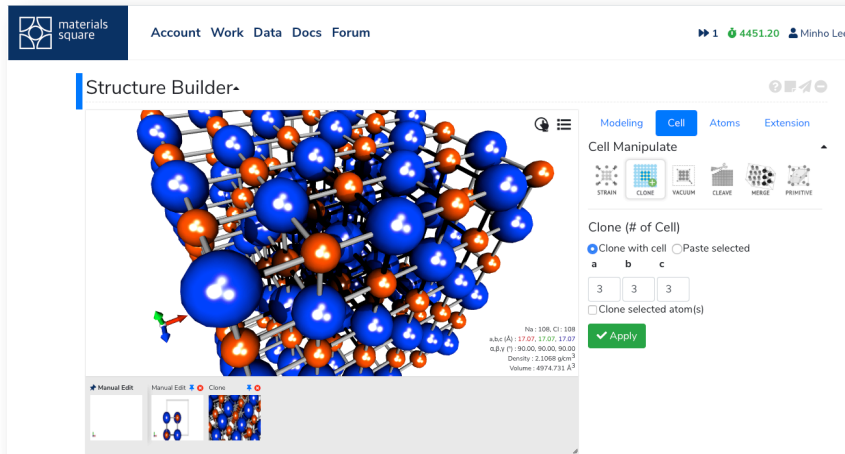
Address 1716, 49, Ahasan-ro 17-gil, Seongdong-gu, Seoul, South Korea

Business Area Web-based Simulation Platform (Materials Square)
Simulation Consulting

New Materials Discovery – Problems



Platform : The SOLUTION

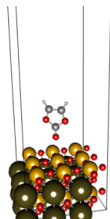


ONLY
Pay-Per-Use
Materials
R&D Platform
(\$0.25/CPU Hour)

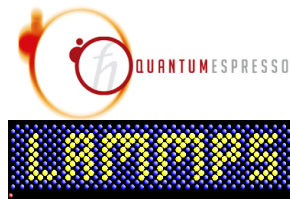
Patent (2017)



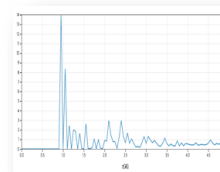
Modeling UI



Simulation Engines



Pre/post processing



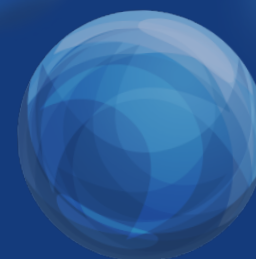
Cloud HPC



Contents

Which Visualizer is Suitable for Your Research?

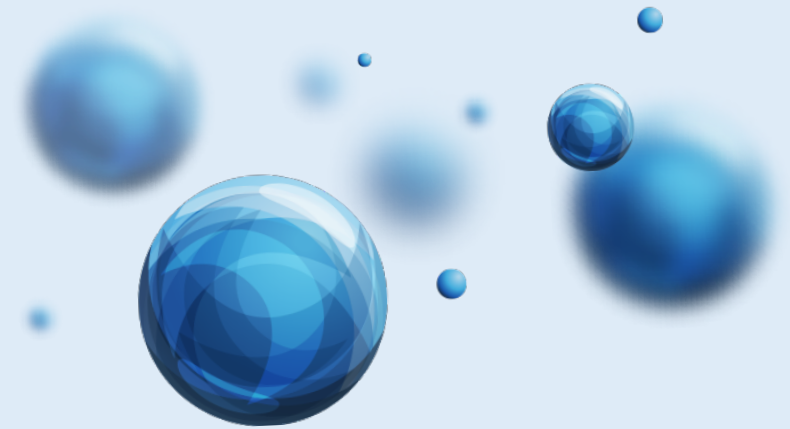
- 1 Introduction
- 2 Structure Visualizer
- 3 Conclusion
- 4 Q & A

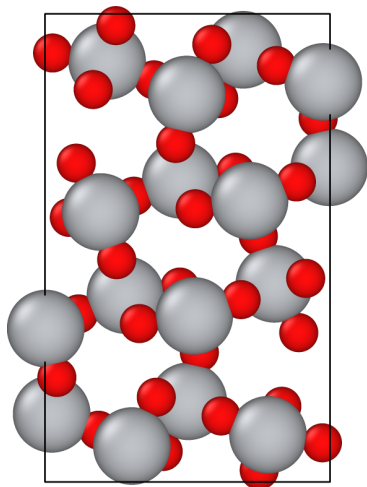


Which Visualizer is Suitable for Your Research?

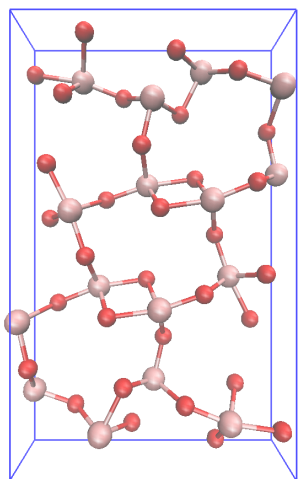
1 Introduction

Which visualizer you used?

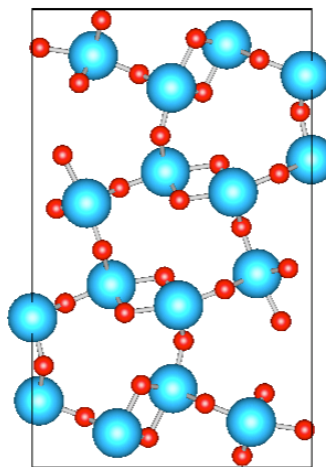




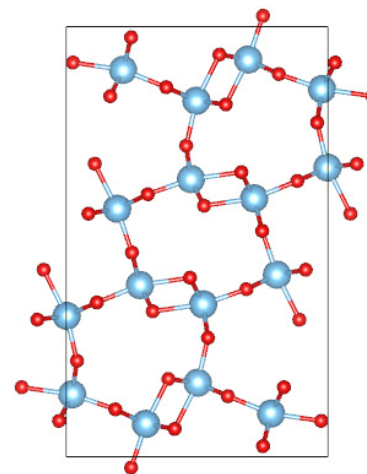
OVITO



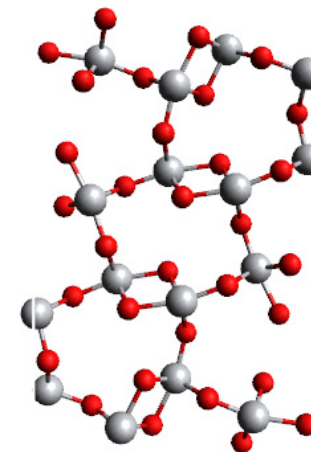
VMD



Materials Square



VESTA



Avogadro

Which Visualizer is Suitable for Your Research?

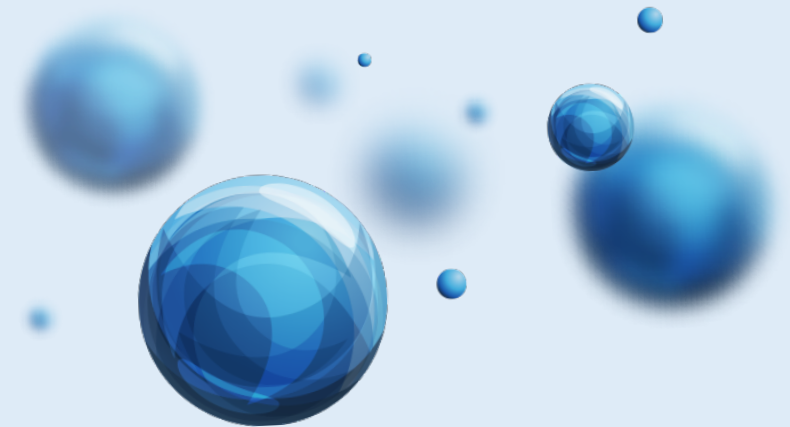
2 Structure visualizer

Visibility

Edit

Analysis

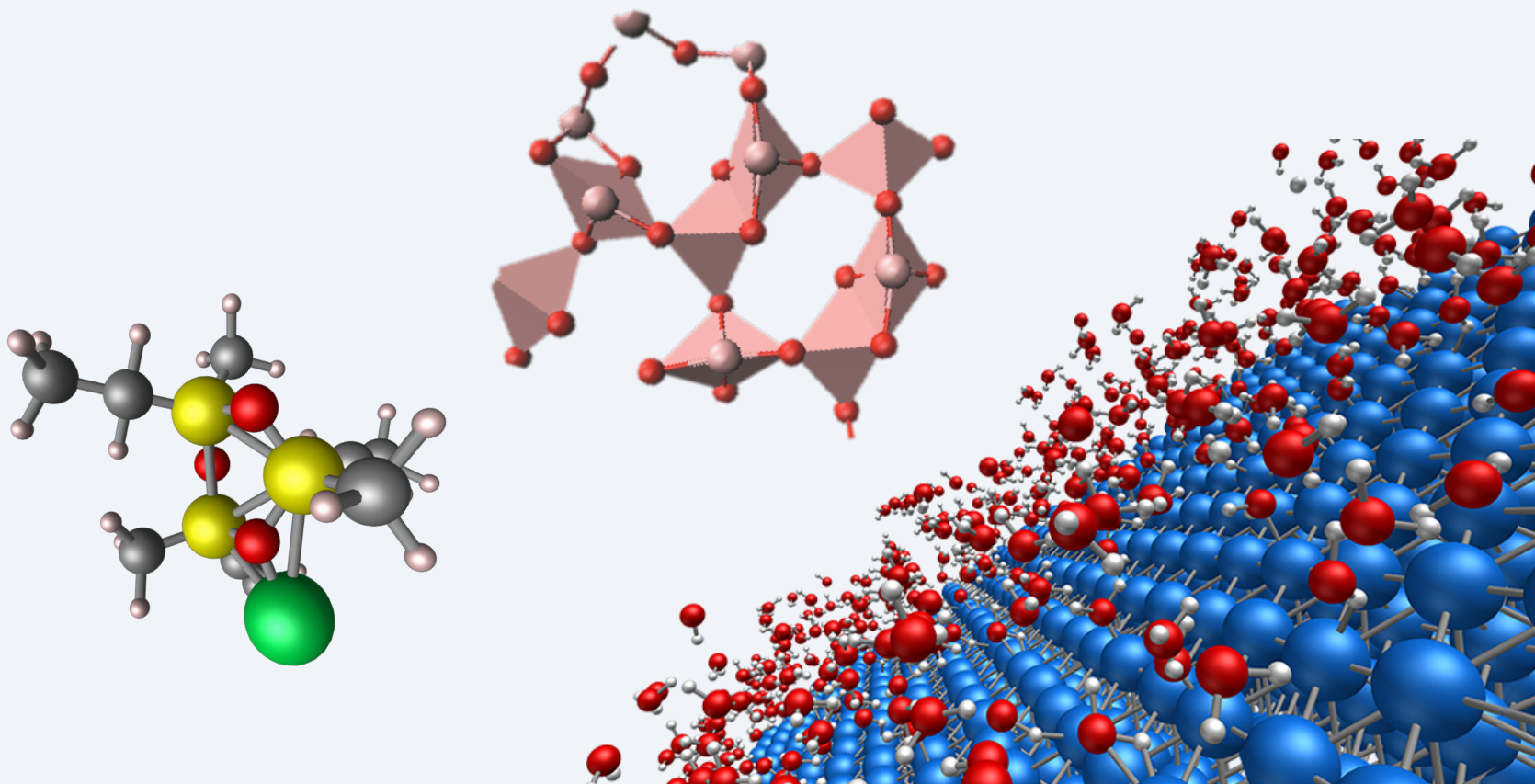
Performance



2 Structure visualizer

Visibility

Which Visualizer is Suitable for Your Research?



Which Visualizer is Suitable for Your Research?

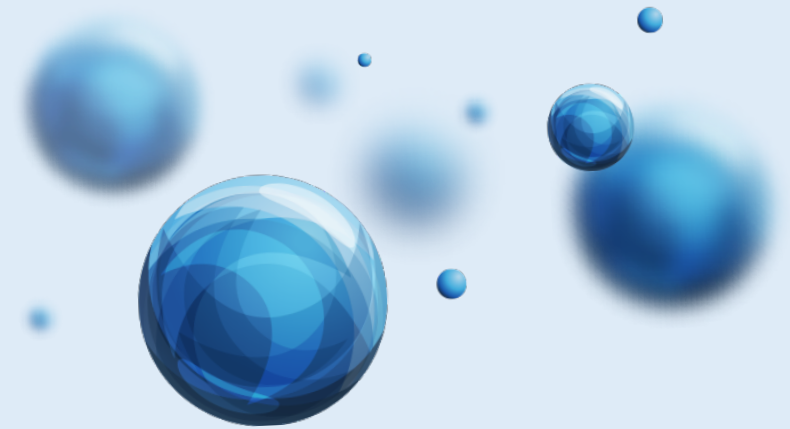
2 Structure visualizer

Visibility

Edit

Analysis

Performance



2 Structure visualizer

Edit



Atom

- › Position/Type
- › Rotation
- › Translation
- › Permutation
- › ...

<https://www.matsq.com>



Lattice (Cell)

- › Lattice Parameters
- › Space/Point Group
- › Clone (supercell)
- › Vacuum
- › Cleave Surface
- › ...

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Bond

- › Bond order
- › Bond type
- › Bond length
- › Charge
- › ...

Which Visualizer is Suitable for Your Research?

2 Structure visualizer

Edit

materials square Account Work Data | Blog Docs | Open Research

\$ 1734.49 0 Log out

Structure Builder

Modeling Cell Atom Extension

DATABASE JOBS MODULE FILE CRYSTAL PRESET EDIT

Search Structure from Open DB

Formula:

ID	Formula	Spacegroup	Natoms	Volume (Å ³)
No result				

Click here to upload structure file
or
Drop your structure file here!

Import Module

Last save: None New Work

<https://www.matsq.com>

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Which Visualizer is Suitable for Your Research?

Database search

Crystal structure search

Don't find crystal structure file

Connect Materials Project Database

2 Structure visualizer

Edit

Structure Builder

Modeling Cell Atom Extension

STRAIN CLONE VACUUM CLEAVE MERGE PRIMITIVE CONVENTIONAL

HISTORY

OpenDB

Conventional

Ti-4, 0-8
a,b,c (Å): 3.80, 3.80, 9.75
α,β,γ (°): 90.00, 90.00, 90.00
Density: 3.765 g/cm³
Volume: 140.958 Å³

Import Module Modeling Simulation Analyzer Etc.

Last save: None New Work Save

Which Visualizer is Suitable for Your Research?

Materials Square's edit feature

Cell Edit (supercell, cleve etc.)

2 Structure visualizer

Edit

materials square Account Work Data | Blog Docs | Open Research ▾ \$ 59

Modeling Cell Atom Extension

ADD ATOM ADD MOLECULE MOVE ROTATE CHANGE

Press ESC key or touch THIS to exit select mode

Select mode - Rectangular Normal

HISTORY

OpenDB ★

H: 24, O: 12
abc (Å): 3.97, 8.12, 8.32
α,β,γ (°): 90.00, 90.00, 90.00
Density: 1.339 g/cm³

<https://www.matsq.com>

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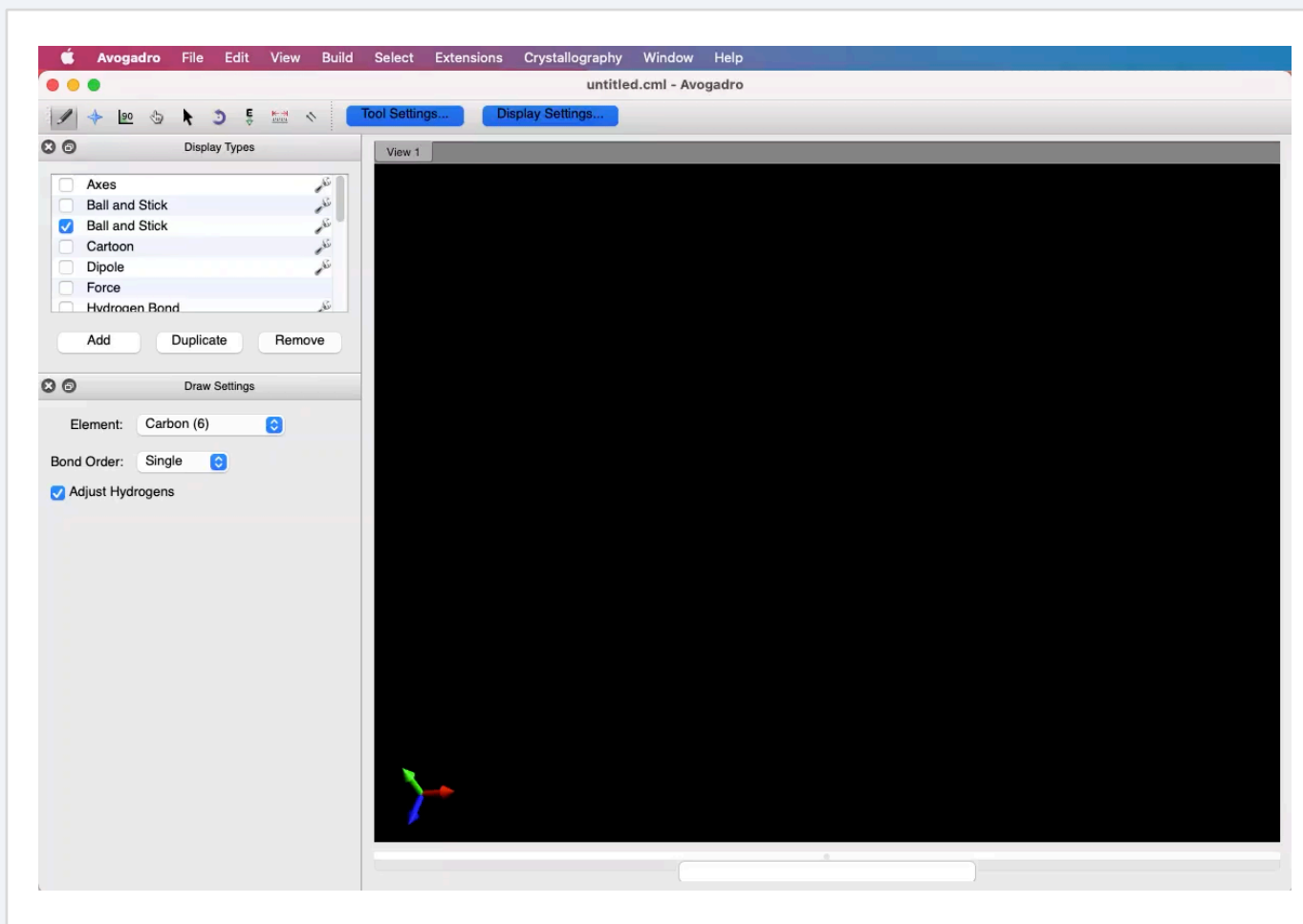
Which Visualizer is Suitable for Your Research?

Materials Square's edit feature

Organic structure builder be
scheduled to February.

2 Structure visualizer

Edit



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Which Visualizer is Suitable for Your Research?

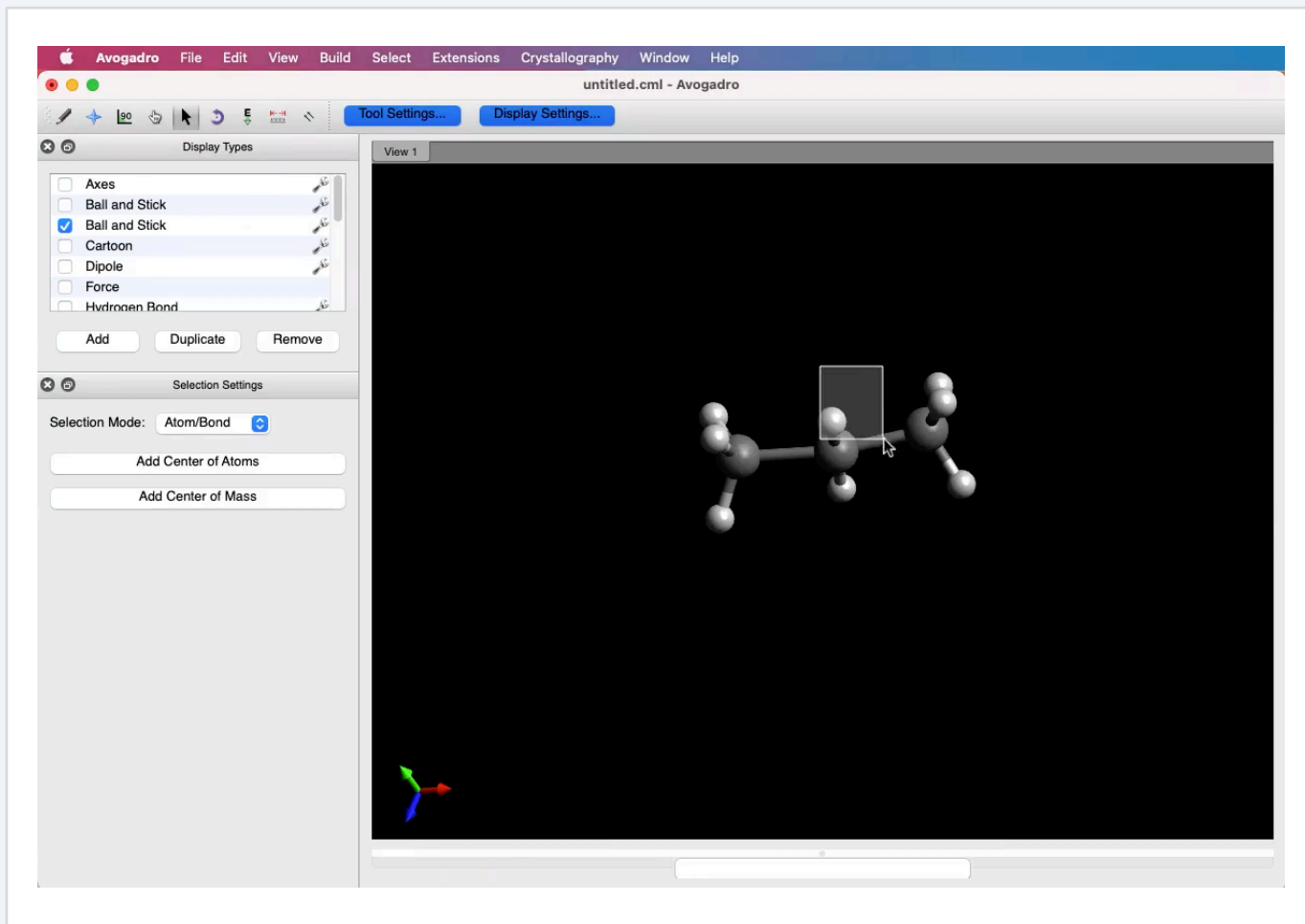
Draw atom

Atom draw using Mouse

Draw with GUI visually easy

2 Structure visualizer

Edit



<https://www.matsq.com>

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Which Visualizer is Suitable for Your Research?

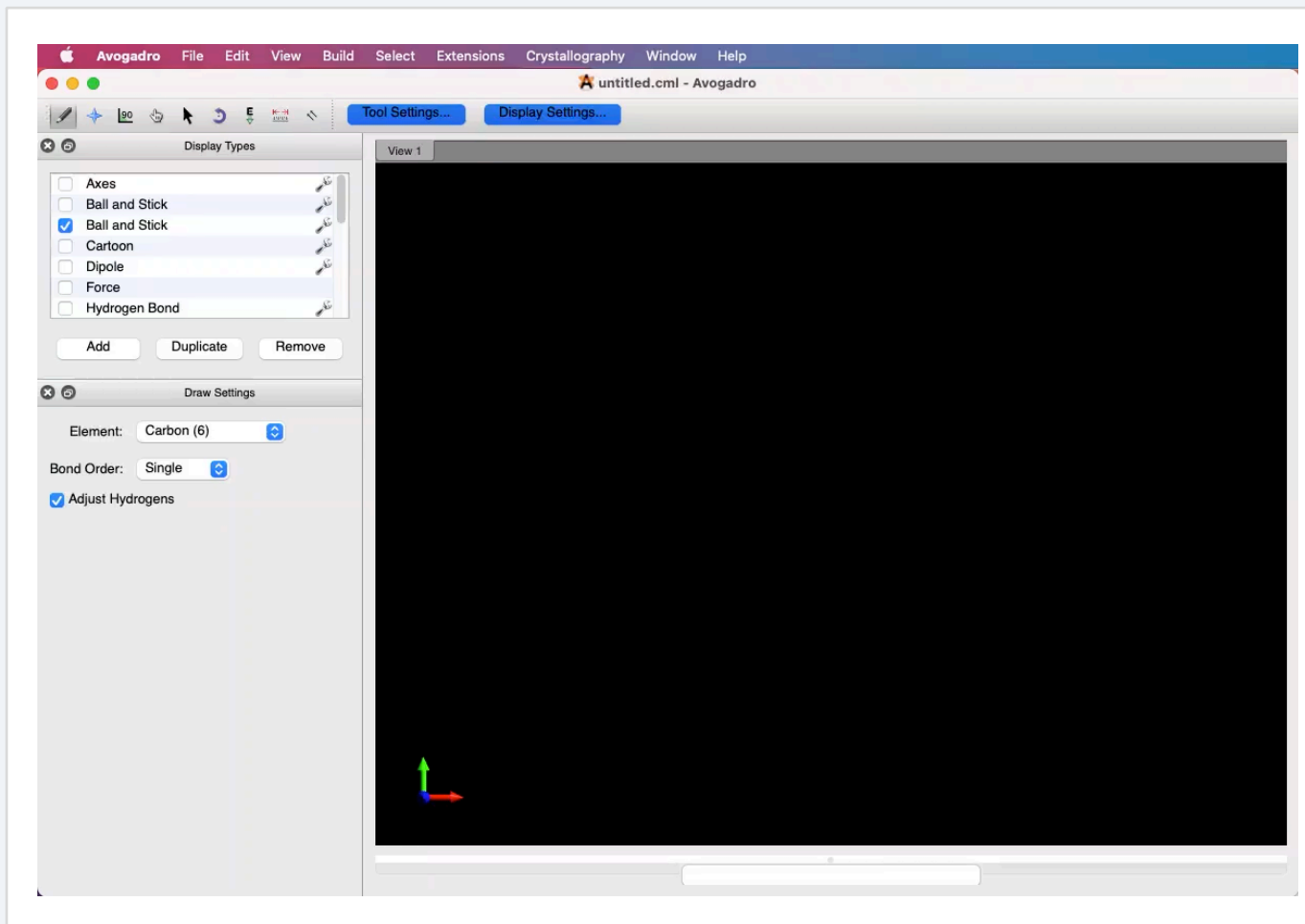
Manipulate edit

Selected atom edit in detail

17

2 Structure visualizer

Edit



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Which Visualizer is Suitable for Your Research?

Conformer search

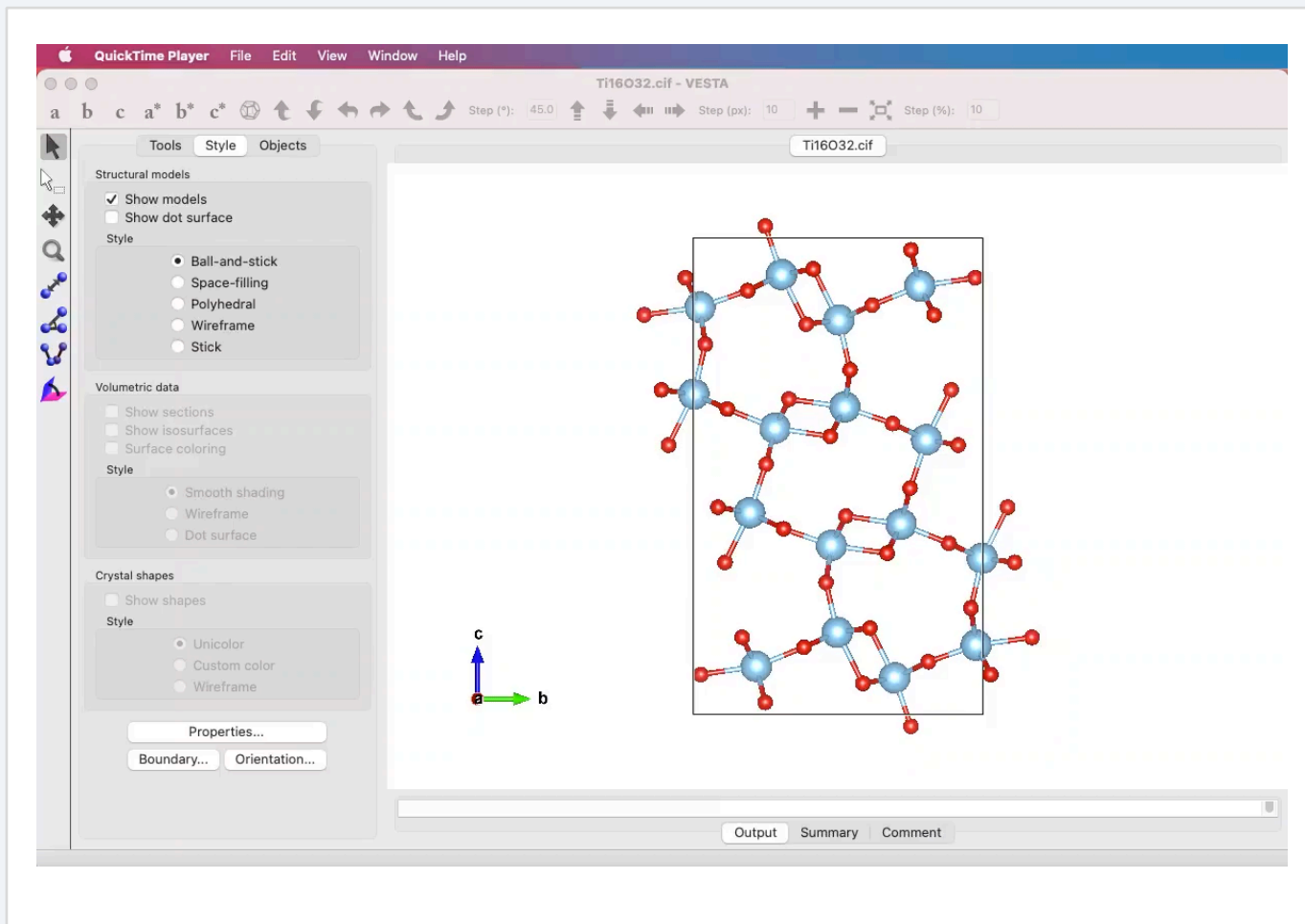
Using inner Forcefield

Roughly drawn structure cleaning

Searching isomer

2 Structure visualizer

Edit



<https://www.matsq.com>

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Which Visualizer is Suitable for Your Research?

Cell transformation

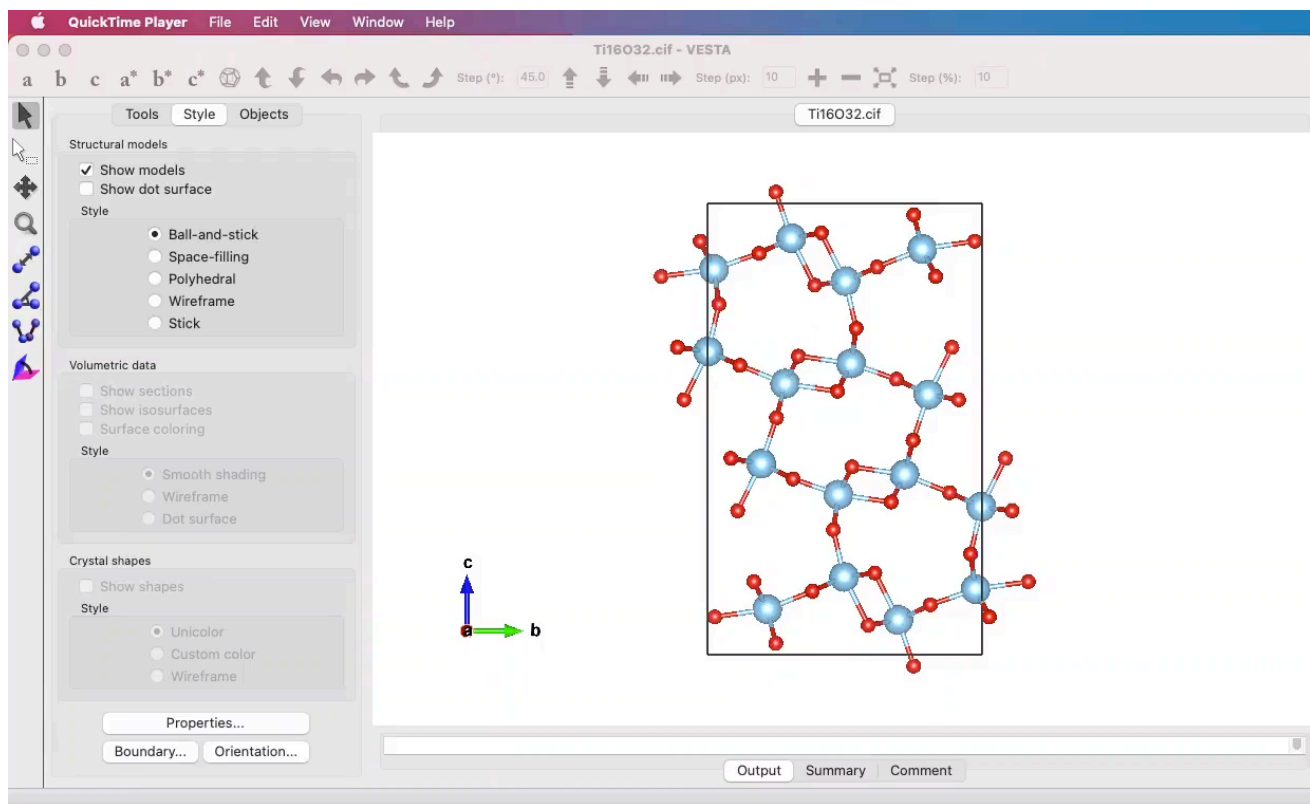
Characterized to inorganic material

Cell transformation

Use manually

2 Structure visualizer

Edit



Which Visualizer is Suitable for Your Research?

Data export

Structure file convert to POSCAR

Calculation Input

Which Visualizer is Suitable for Your Research?

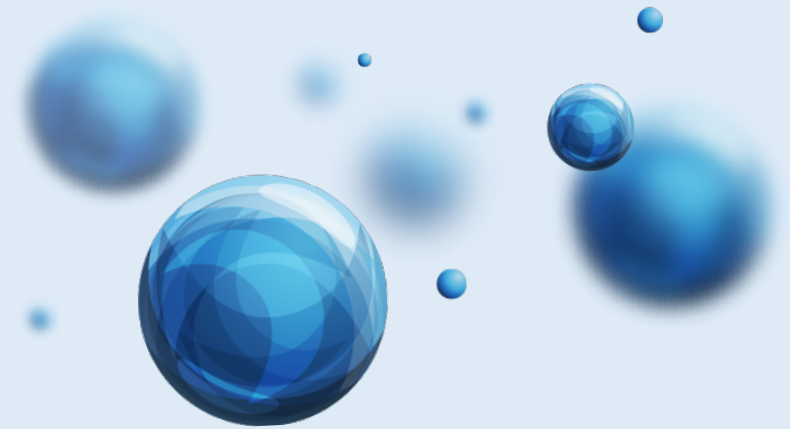
2 Structure visualizer

Visibility

Edit

Analysis

Performance



2 Structure visualizer

Analysis

Which Visualizer is Suitable for Your Research?



Electronic structure

- › Density of States
- › Charge density
- › Band structure
- › Orbital surface
- › ...

<https://www.matsq.com>



Atomic structure

- › RDF
- › Defects
- › Dislocation analysis
- › Voronoi analysis
- › ...

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Energetics

- › Total Energy
- › Binding Energy
- › Gibbs Free Energy
- › ...

22

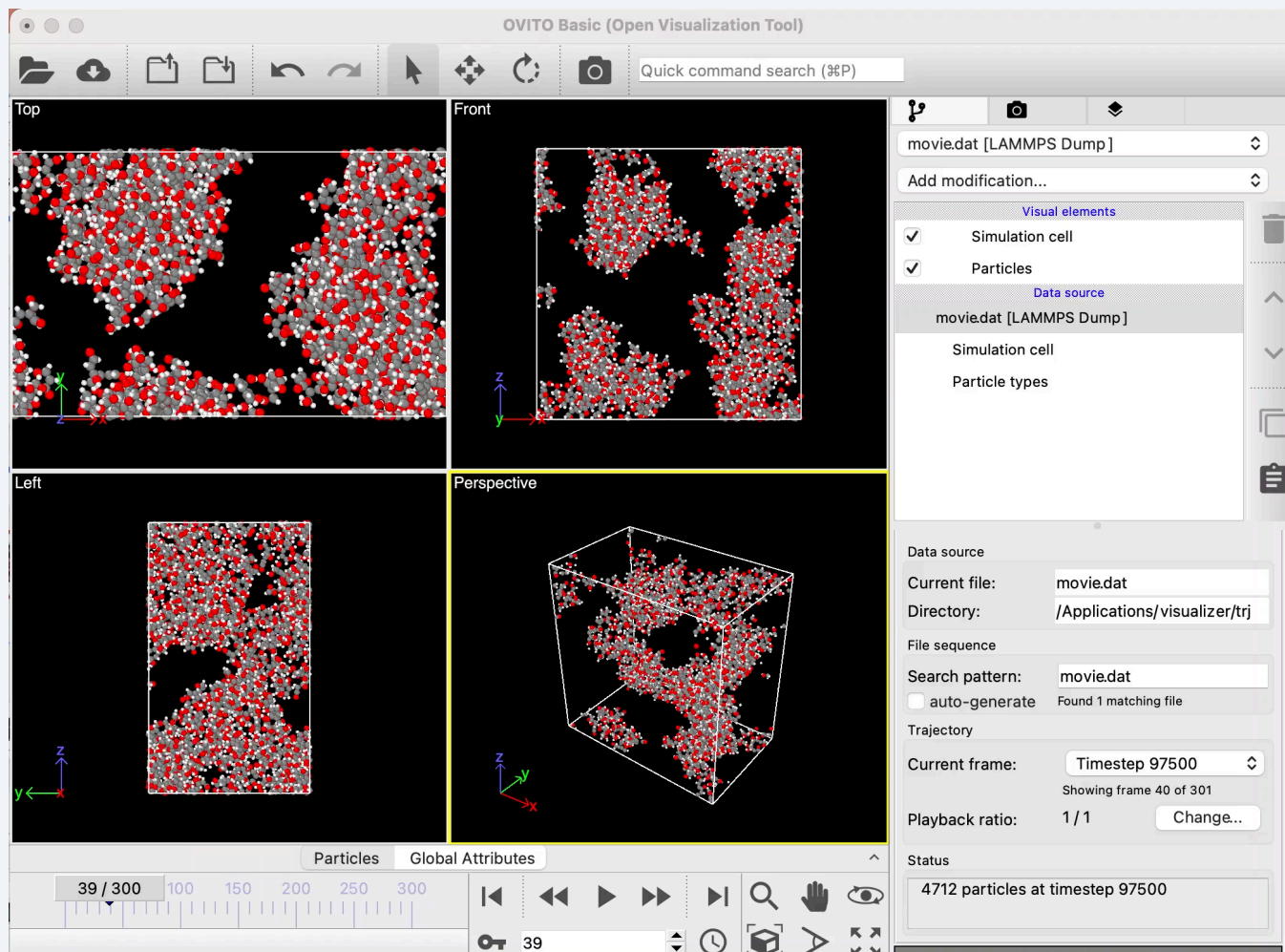
2 Structure visualizer

Analysis

Which Visualizer is Suitable for Your Research?

RDF

Analysis radial distribution function



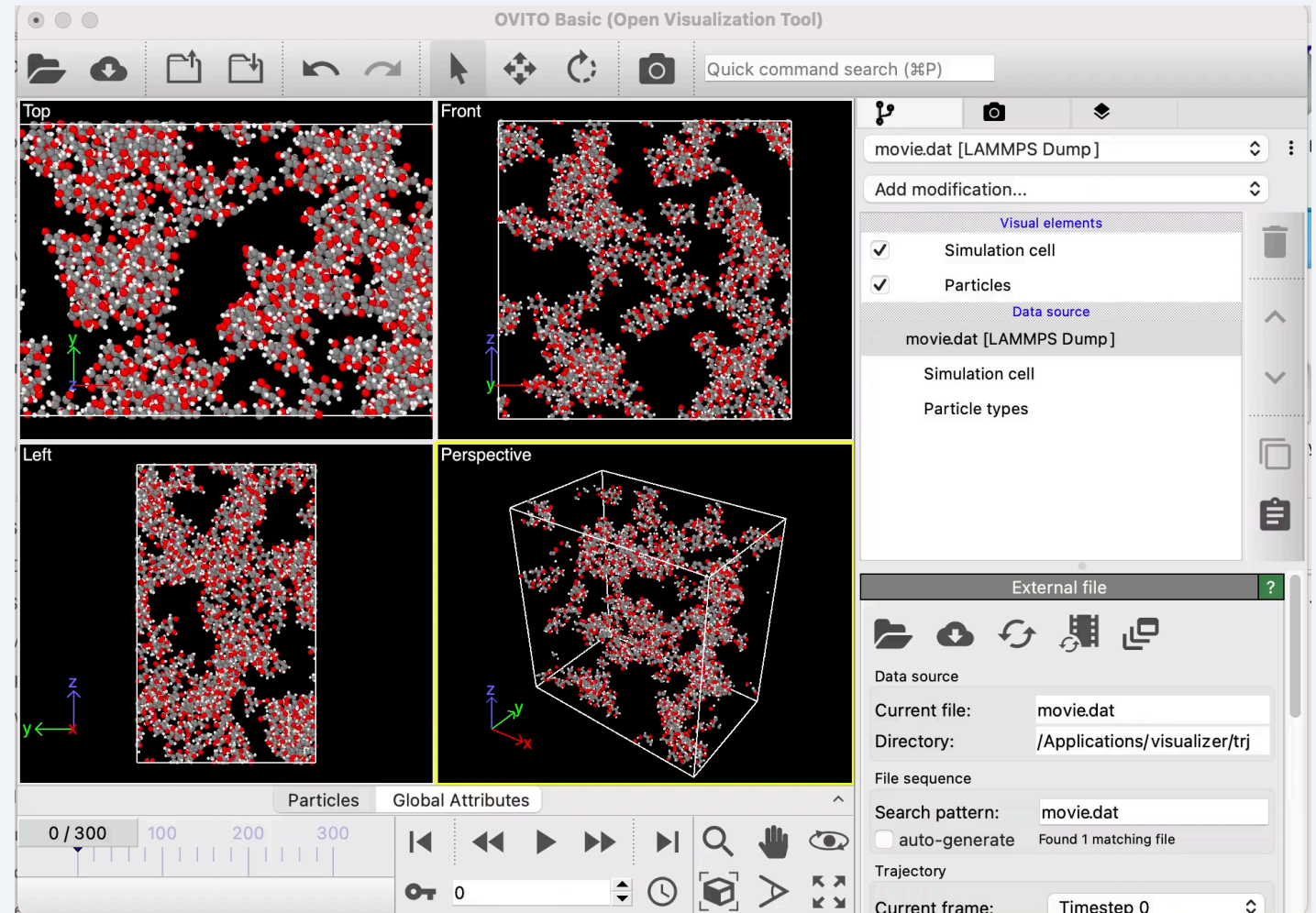
2 Structure visualizer

Analysis

Cluster analysis

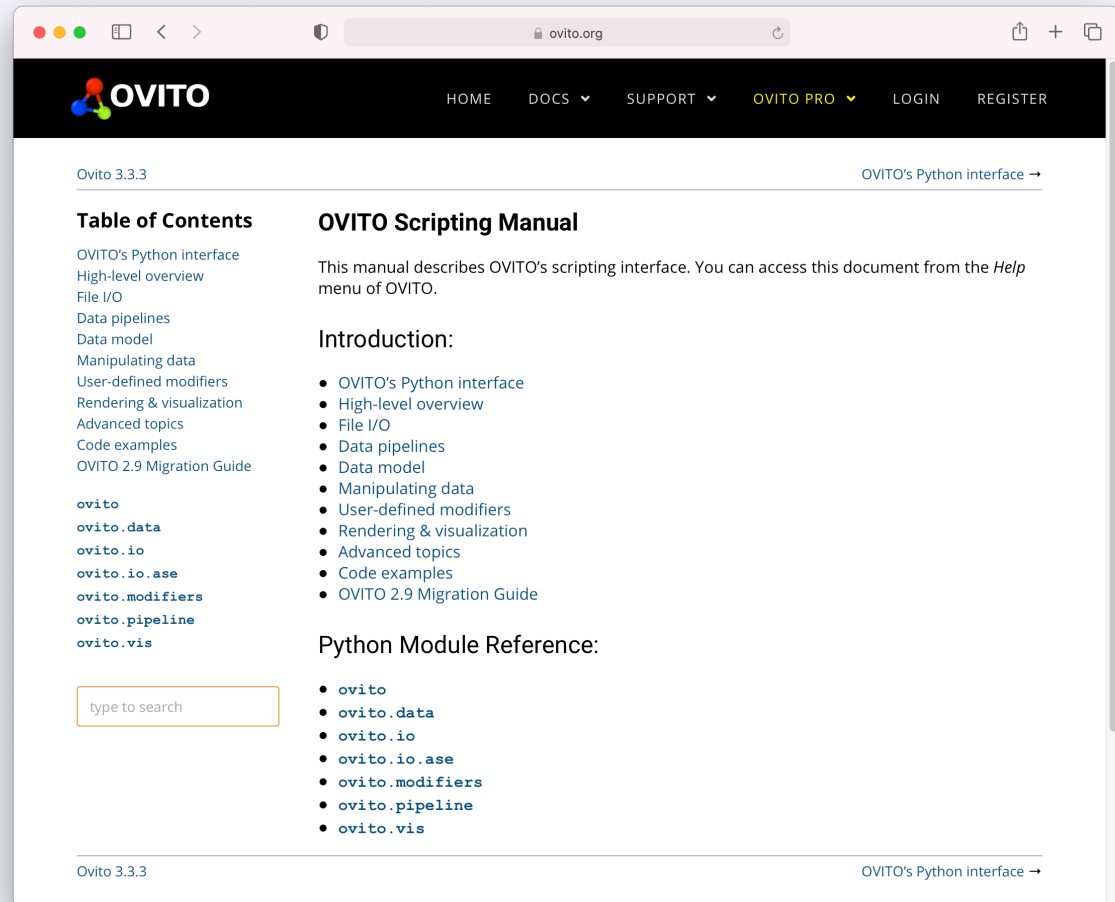
Analysis how many cluster in system

Which Visualizer is Suitable for Your Research?



OVITO (Python interface)

- Automate data visualization and analysis steps.
- Integrate OVITO's data I/O, analysis and rendering capabilities into custom workflows or Python programs.
- Extend OVITO capabilities by developing new modifiers or viewports layers that integrate into the graphical user interface.



The screenshot shows the OVITO website's Python interface documentation page. The page is titled "OVITO 3.3.3" and "OVITO's Python interface". It features a navigation bar with links for HOME, DOCS, SUPPORT, OVITO PRO, LOGIN, and REGISTER. The main content is divided into two columns. The left column contains a "Table of Contents" with links to various sections: OVITO's Python interface, High-level overview, File I/O, Data pipelines, Data model, Manipulating data, User-defined modifiers, Rendering & visualization, Advanced topics, Code examples, and OVITO 2.9 Migration Guide. Below the table of contents is a search box labeled "type to search". The right column is titled "OVITO Scripting Manual" and contains an "Introduction" section with a bulleted list of links to the same sections as the table of contents. Below the introduction is a "Python Module Reference" section with a bulleted list of links to the same sections. The page also includes a footer with "OVITO 3.3.3" and "OVITO's Python interface" links.

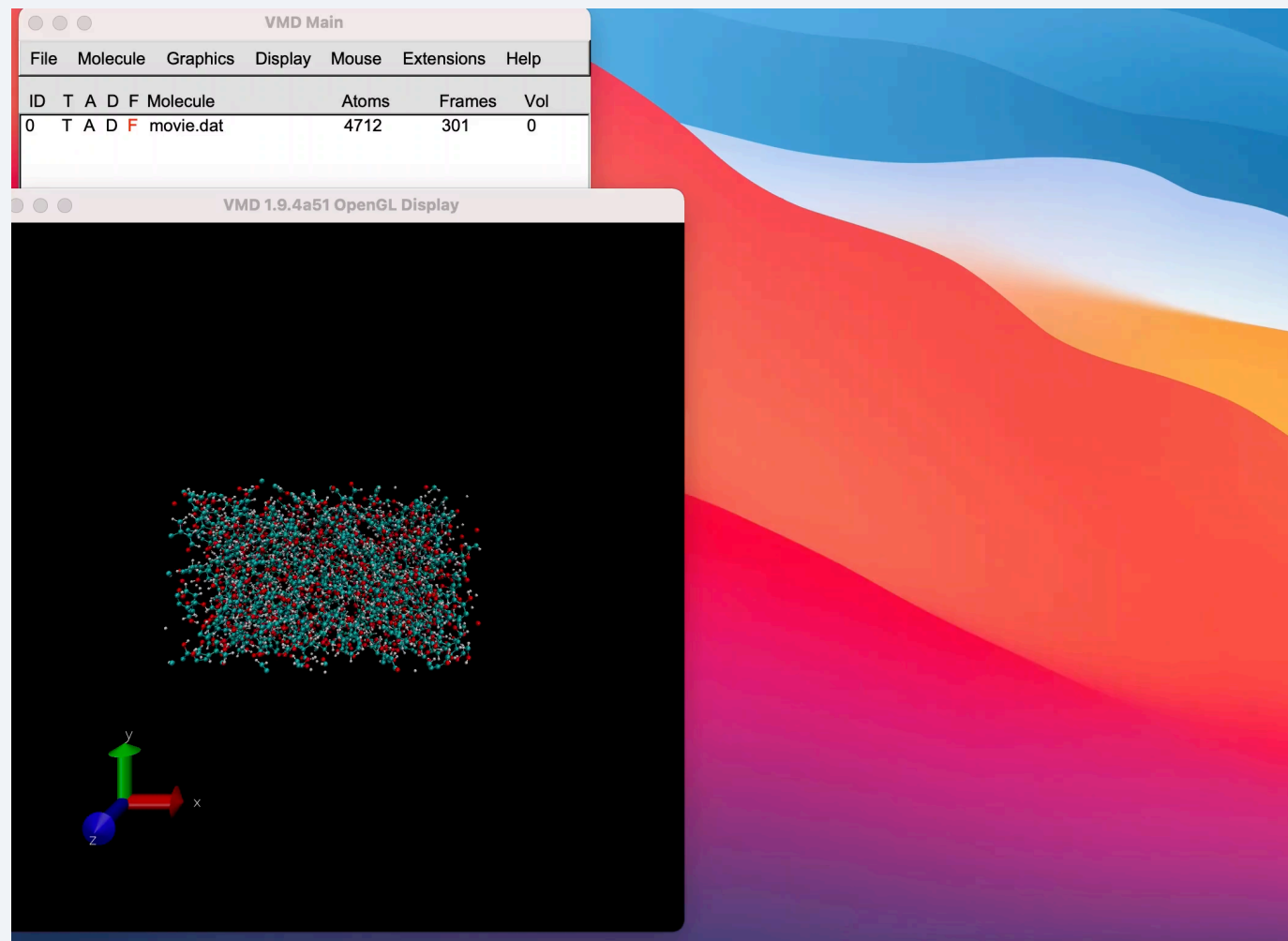
2 Structure visualizer

Analysis

Which Visualizer is Suitable for Your Research?

RDF

Analysis radial distribution
function



VMD (Tk console)

- VMD provides embedded scripting languages (Python and Tcl) for the purpose of user extensibility.

Previous

Next: [Data Analysis in VMD](#) Up: [VMD Tutorial](#) Previous: [Trajectories and Movie Making](#)

Subsections

- [The Basics of Tcl Scripting](#)
- [VMD scripting](#)
 - [Loading molecules with text commands](#)
 - [The atomelect command](#)
 - [Obtaining and changing molecule properties with text commands](#)
 - [Sourcing scripts](#)
- [Drawing shapes](#)

Scripting in VMD

VMD provides embedded scripting languages (Python and Tcl) for the purpose of user extensibility. In this section we will discuss the basic features of the Tcl scripting interface in VMD. You will see that everything you can do in VMD interactively can also be done with Tcl commands and scripts, and how the extensive list of Tcl text commands can help you investigate molecule properties and perform analysis.

The Basics of Tcl Scripting

To execute Tcl commands, you will be using a convenient text console called *Tk Console*.

- 1 Start a new VMD session. In the VMD Main menu select *Extensions* → *Tk Console* to open the *VMD TkConsole* window (Fig. 21). You can now start entering Tcl/Tk commands here.

2 Structure visualizer

Analysis

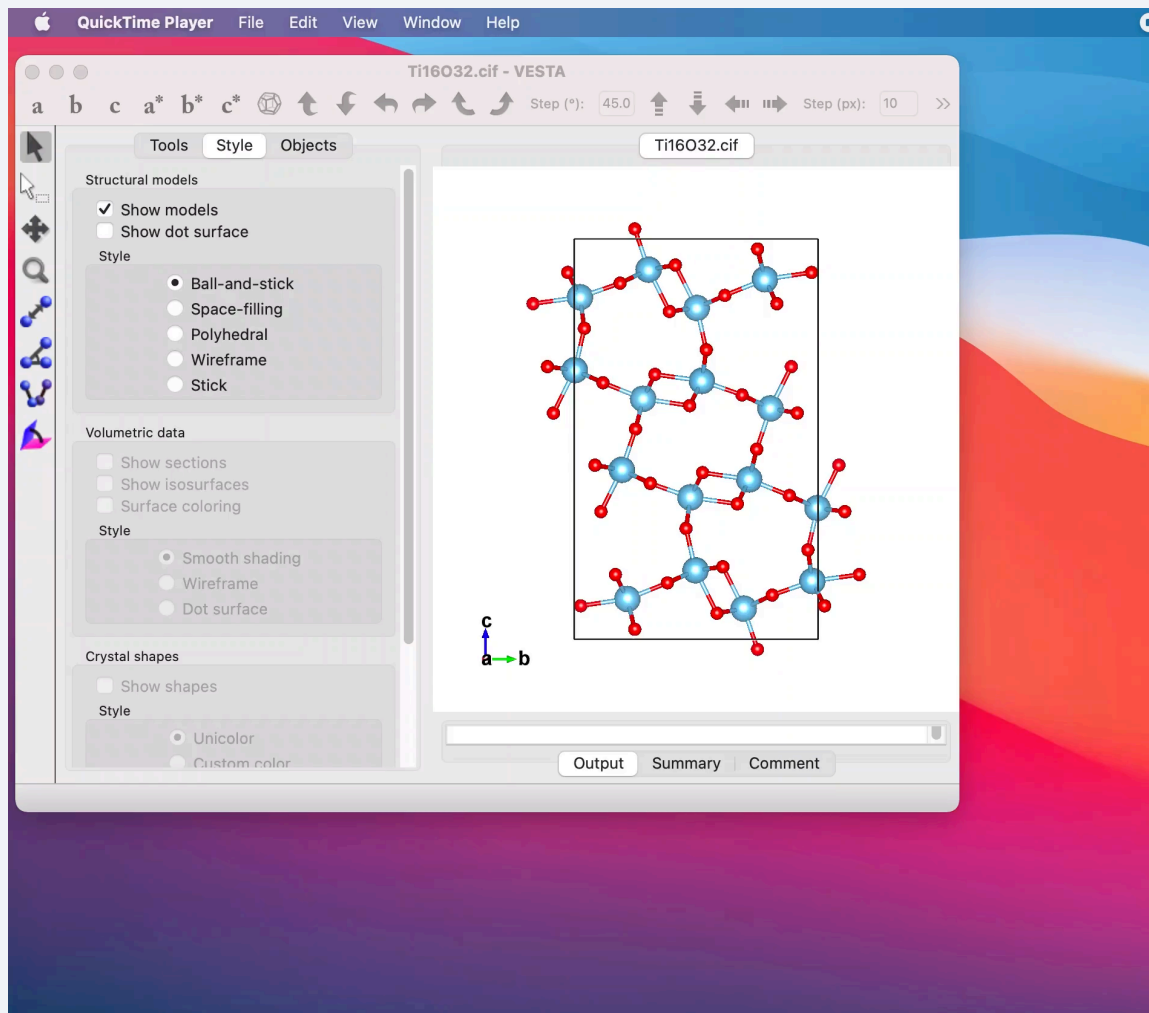
Which Visualizer is Suitable for Your Research?

VESTA (XRD pattern)

XRD pattern

Set source wavelength

Crystal information



2 Structure visualizer

Analysis

Which Visualizer is Suitable for Your Research?

MatSQ (Charge Density)

Charge density observe

MatSQ (Simulated STM)

Simulated STM image observe

The screenshot displays the Materials Square web interface. At the top, there is a navigation bar with the Materials Square logo and links for Account, Work, Data, Blog, Docs, and Open Research. The user's account balance is shown as \$ 5052.33, and there is a Log Out button.

The main content area is divided into two sections:

- Charge Density:** This section shows a 3D visualization of a charge density difference. The structure is a chain of atoms with a red sphere representing a charge density peak. The formula is $+p1 - p2 - p3$. A color scale on the right ranges from -0.195 to 0.321 e/bohr³. A tooltip for the Isovalue shows 0.1 e/bohr³ with a color type of Plane BGR and a scale from -0.194650 to 0.3209392. A Redraw button is present.
- Quantum Espresso:** This section shows the simulation settings. It indicates that the simulation is "Successfully finished (id : 35481)". The settings include:
 - PWscf, Charge Density, and DOS are selected.
 - Scripting Option: Template
 - Update Structure:
 - Data to get: Charge Density
 - Precision: High (long time)
 - Model type: Isolate System
 - Structure optimization: No optimization
 - Options: Spin polarization (checked), Van der Waals, Electric field, Spin Orbit Coupling, and DFT+U.

At the bottom, there is a footer with "Import Module", "Structure Builder", "Simulation", "Analyzer", and "Etc." buttons. The last save time is 2020-08-18 13:41:44, and the current view is "Charge Density Difference". A Save button and a settings icon are also visible.

Which Visualizer is Suitable for Your Research?

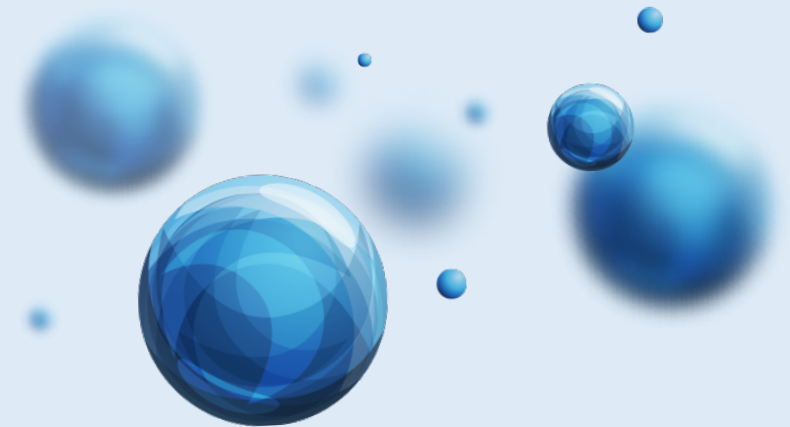
2 Structure visualizer

Visibility

Edit

Analysis

Performance



Benchmark Device Hardware

Hardware Overview:

Model Name:	MacBook Pro
Model Identifier:	MacBookPro16,2
Processor Name:	Quad-Core Intel Core i5
Processor Speed:	2 GHz
Number of Processors:	1
Total Number of Cores:	4
L2 Cache (per Core):	512 KB
L3 Cache:	6 MB
Hyper-Threading Technology:	Enabled
Memory:	16 GB

Visualizer Benchmark test 1

CPK Style representation

No bonding, only ball with default value

Visualizer Benchmark test 2

Bonding style representation

No balls, Only bonding with default value

Visualizer Benchmark (atom drawing)

CPU Usage(%)

# of Atoms	VMD	VESTA	Avogadro	OVITO	MatSQ
1 K	32.1	19.0	17.9	18.6	18.1
10 K	48.3	16.9	18.6	18.3	18.5
20 K	47.5	15.9	17.4	18.4	18.3
40 K	45.8	16.8	19.2	18.7	18.3
80 K	59.4	18.1	18.0	18.6	18.3
100 K	45.6	Can't load	18.4	19.5	19.0

Mem Usage(%)

# of Atoms	VMD	VESTA	Avogadro	OVITO	MatSQ
1 K	0.7	0.2	0.2	0.2	0.2
10 K	0.7	0.2	0.2	0.2	0.2
20 K	0.7	0.2	0.2	0.2	0.2
40 K	0.8	0.2	0.2	0.2	0.2
80 K	0.9	0.2	0.2	0.2	0.2
100 K	1.0	Can't load	0.2	0.2	0.2

Performance

Visualizer Benchmark (bond drawing)

CPU Usage(%)

# of Atoms	VMD	VESTA
1 K	47.1	16.6
10 K	47.4	16.1
20 K	47.8	16.6
40 K	48.8	16.7
80 K	49.5	18.0
100 K	47.8	Can't load

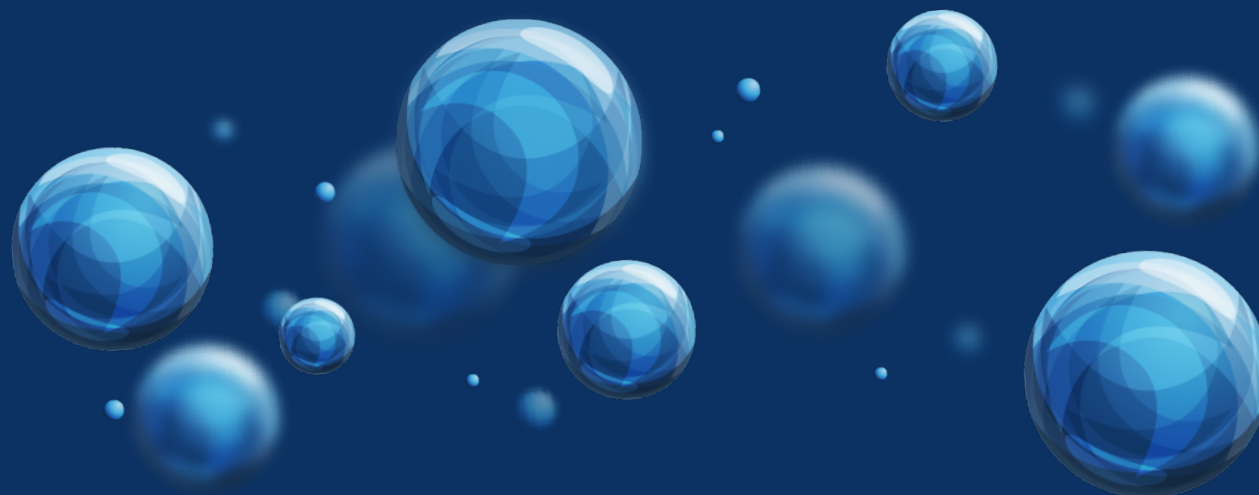
Mem Usage(%)

# of Atoms	VMD	VESTA
1 K	0.8	0.2
10 K	1.3	0.2
20 K	1.7	0.2
40 K	3.8	0.2
80 K	14.7	0.2
100 K	23.6	Can't load

- **Combine several visualizer's features**
- **Make your visualizer skill**
- **Your suitable visualizer made by You**

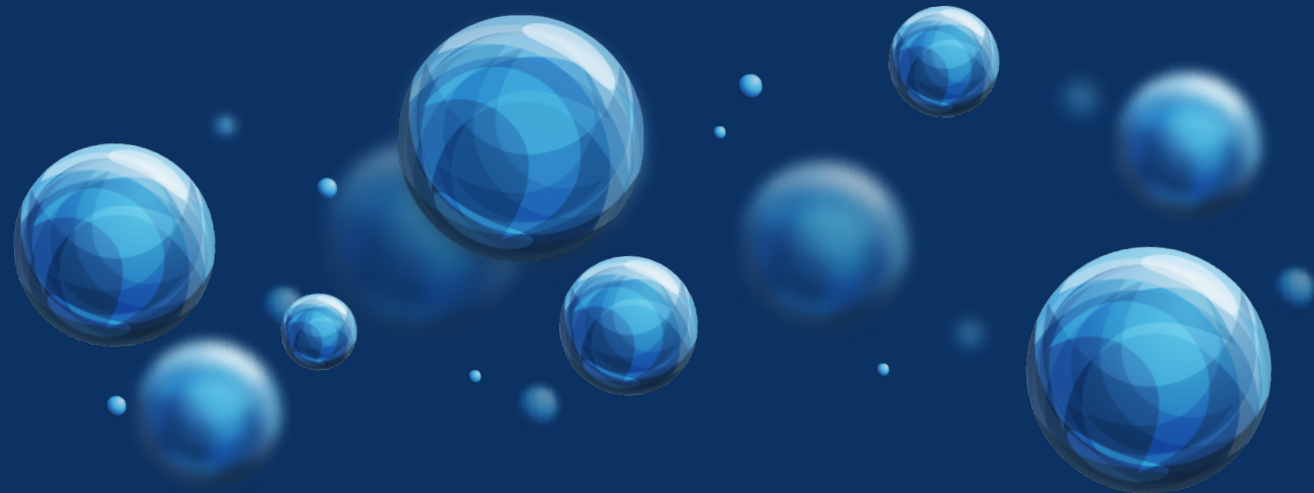
Q & A

- END -





Appendix



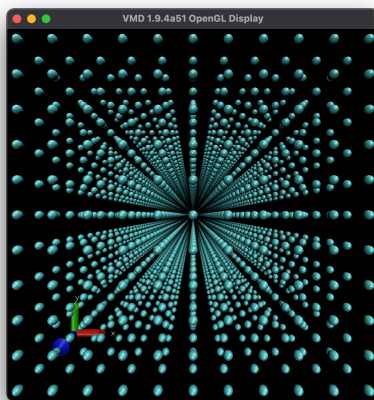
Prepare test structure set

<Avogadro>

1. Draw C atom in the Avogadro window
2. Add Unitcell
3. Supercell build (to 1K, 10K, 20K, 40K, 80K, 100K atoms)
4. Export to xyz file

<All visualizer>

1. Import test set
2. Measure CPU, Memory, FPS



Test example

Visualizer Benchmark test 1

CPK Style representation

No bonding, only ball with default value

Visualizer Benchmark test 2

Bonding style representation

No balls, Only bonding with default value