materials square

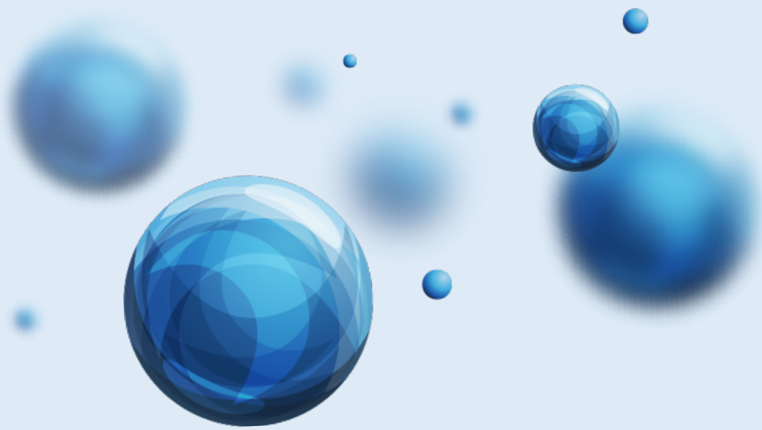
Which Visualizer is Suitable for Your Research?

Speaker : Kyungyeol Gu

Virtual Lab. Inc.

0 About us

About us



ABOUT US

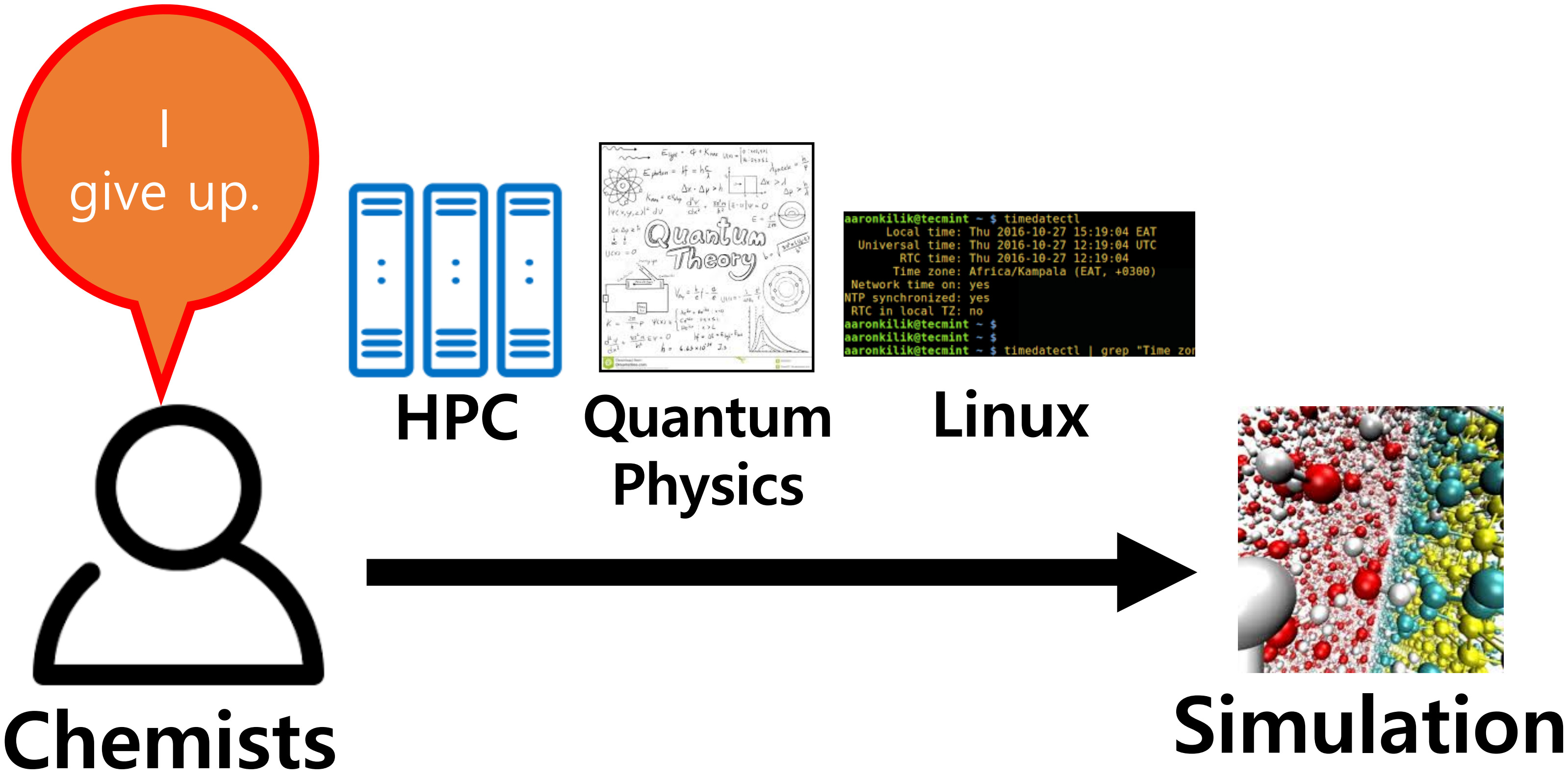
Introduction

Members

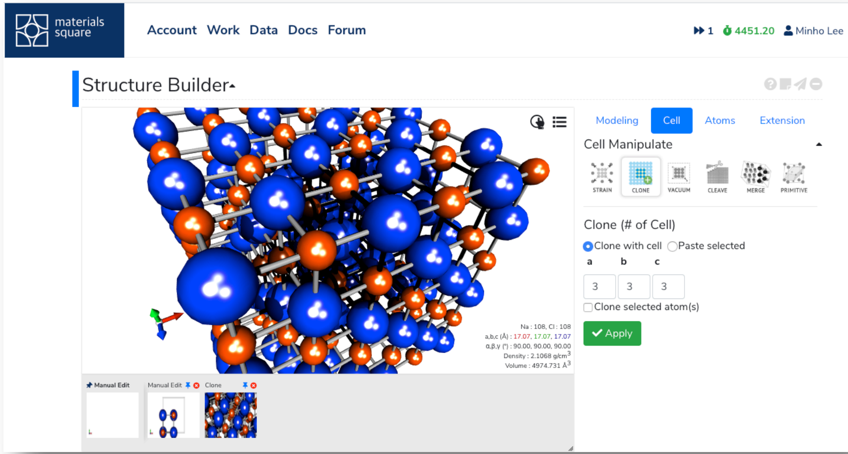
We started this business to break barriers and help everyone do their own simulation in easy-to-learn and user-friendly web environment.
Our proprietary web-based simulation service 'Materials Square', designed with an intuitive interface to the computing environment of the cloud server, provides a 'comprehensive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

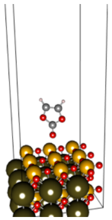
Materials

R&D Platform

($0.25/CPU Hour)

Patent (2017)

Modeling UI

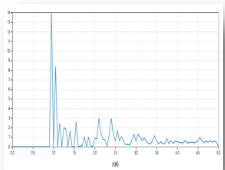


Simulation Engines

QUANTUMESPRESSO

LAMMPS

Pre/post processing

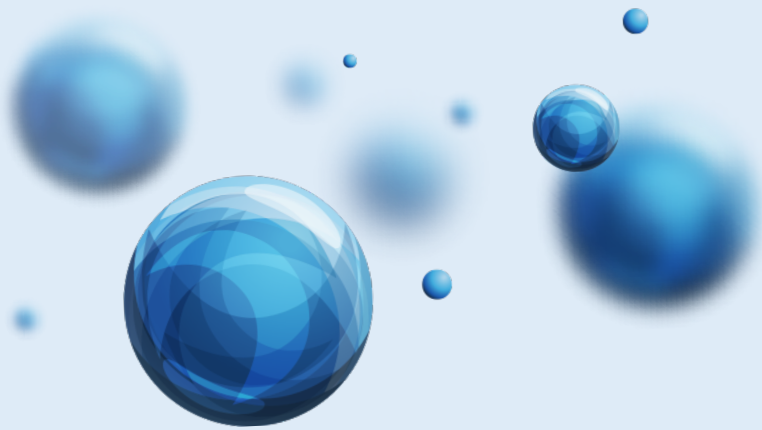


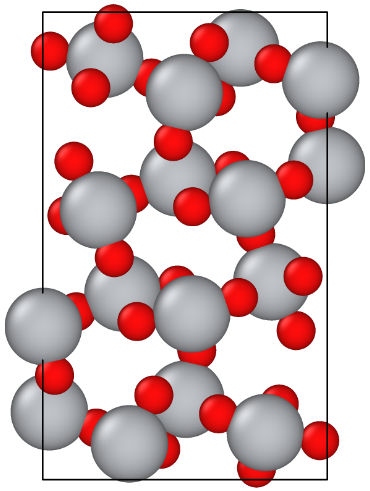
Cloud HPC

Contents

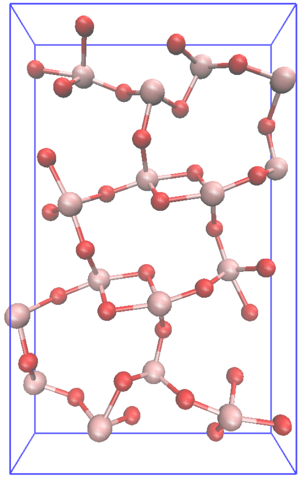
1 Introduction

Which visualizer you used?

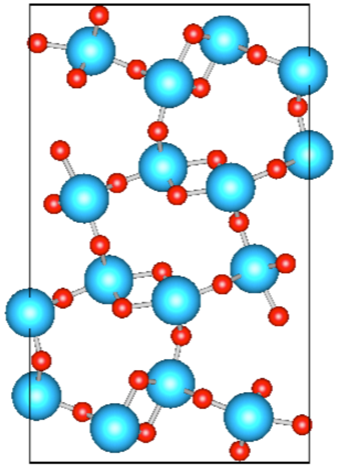




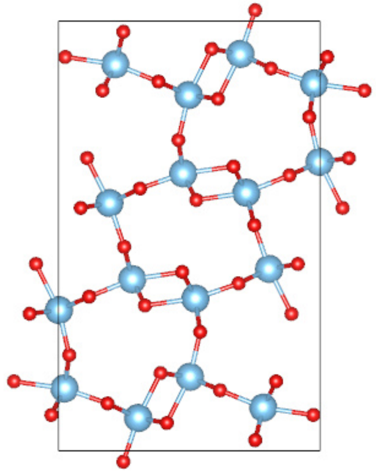
OVITO



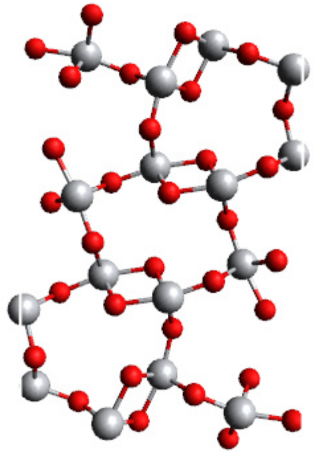
VMD



Materials Square



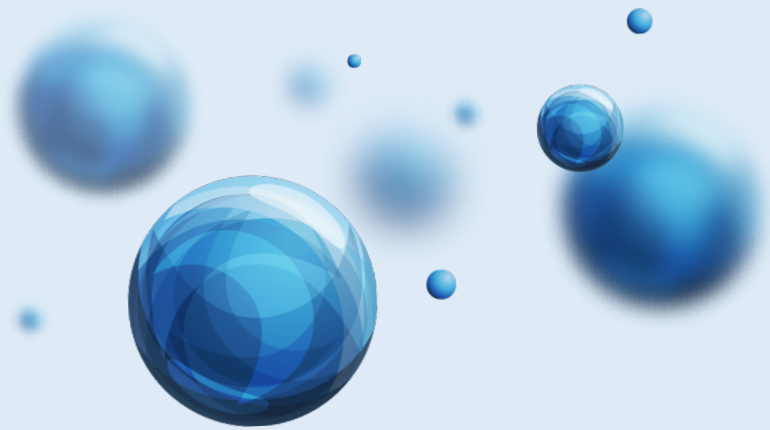
VESTA



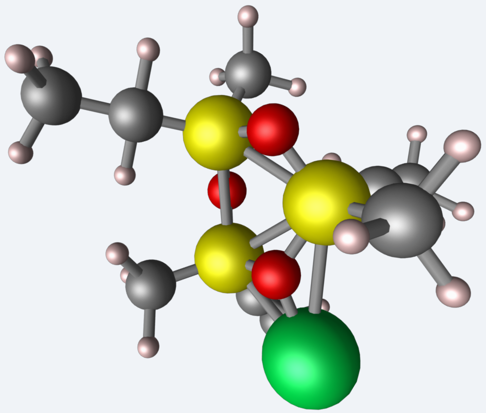
Avogadro

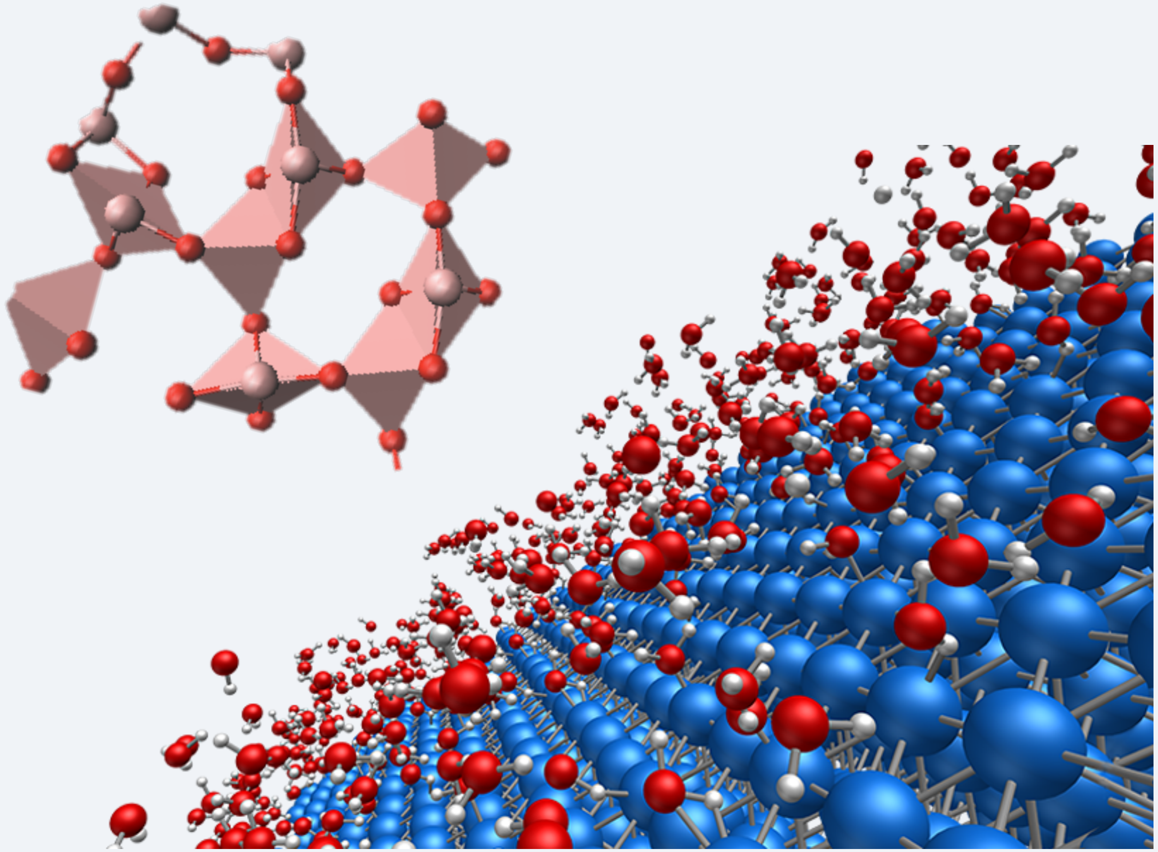
2 Structure visualizer

- **Visibility**
- Edit
- Analysis
- Performance



Visibility





2 Structure visualizer

- Visibility
- **Edit**
- Analysis
- Performance

Edit

Atom

- Position/Type
- Rotation
- Translation
- Permutation
- …

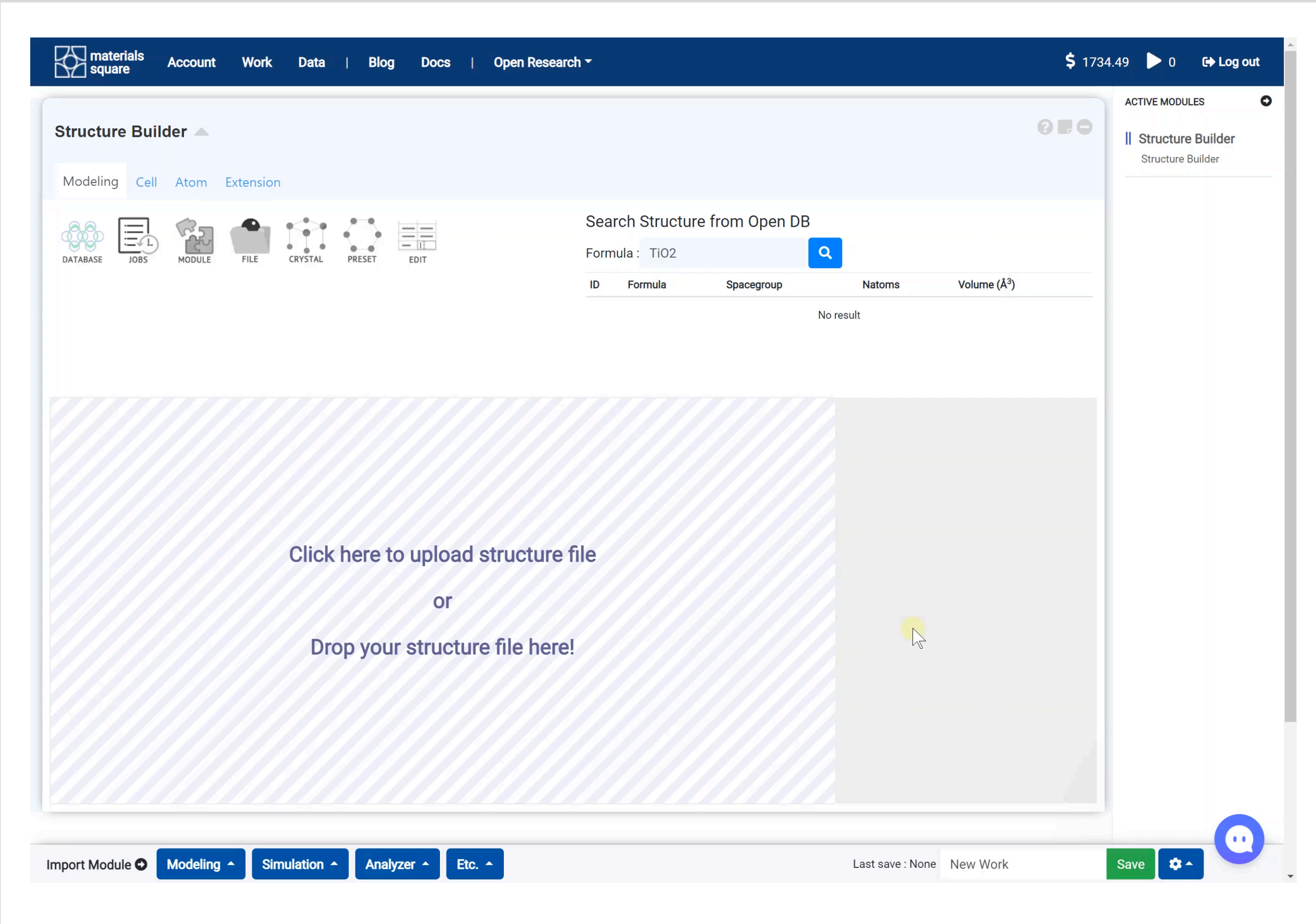
Lattice (Cell)

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

Bond

- Bond order
- Bond type
- Bond length
- Charge
- …

Edit



Database search

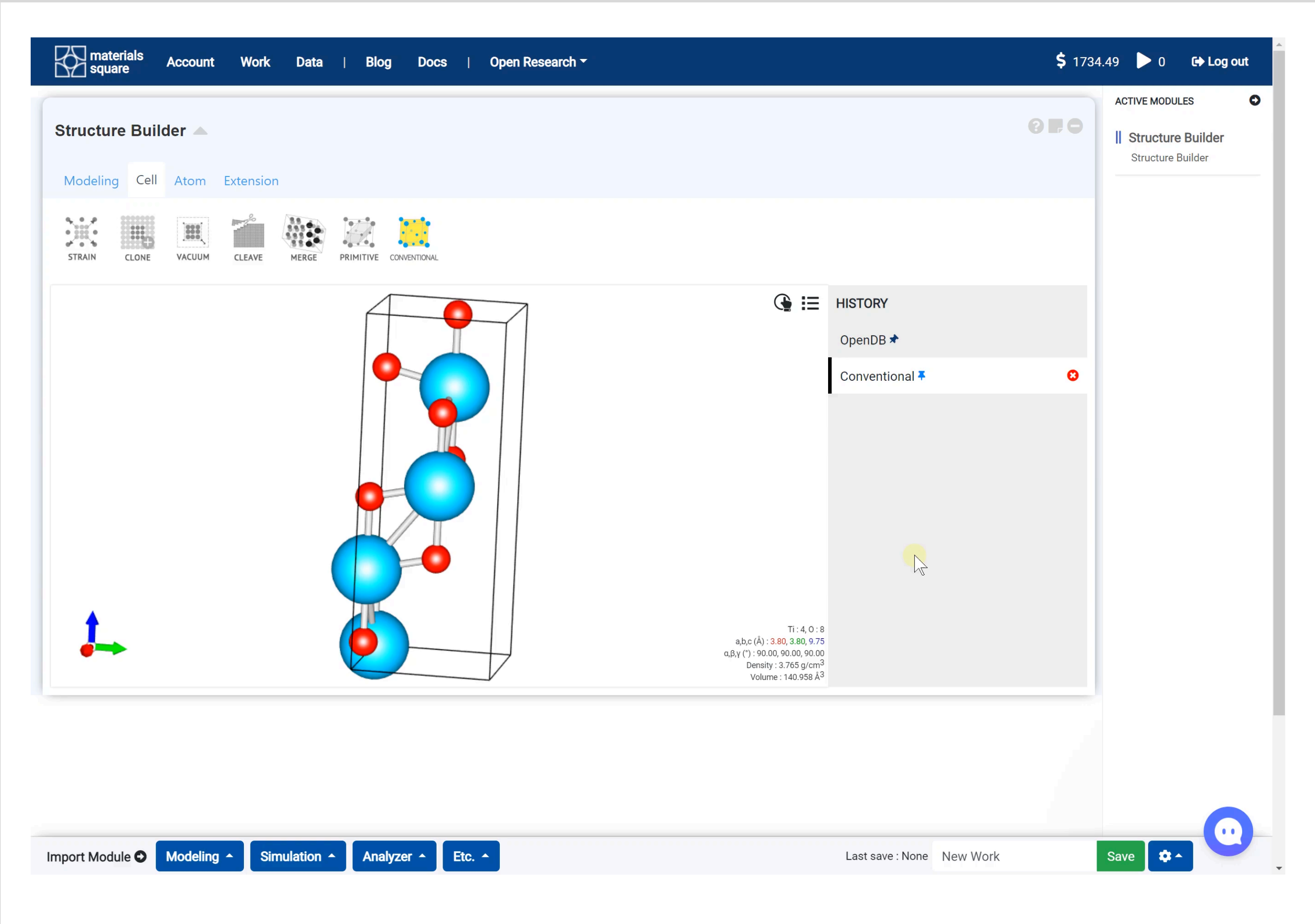
Crystal structure search

Don’t find crystal structure file

Connect Materials Project Database

2 Structure visualizer

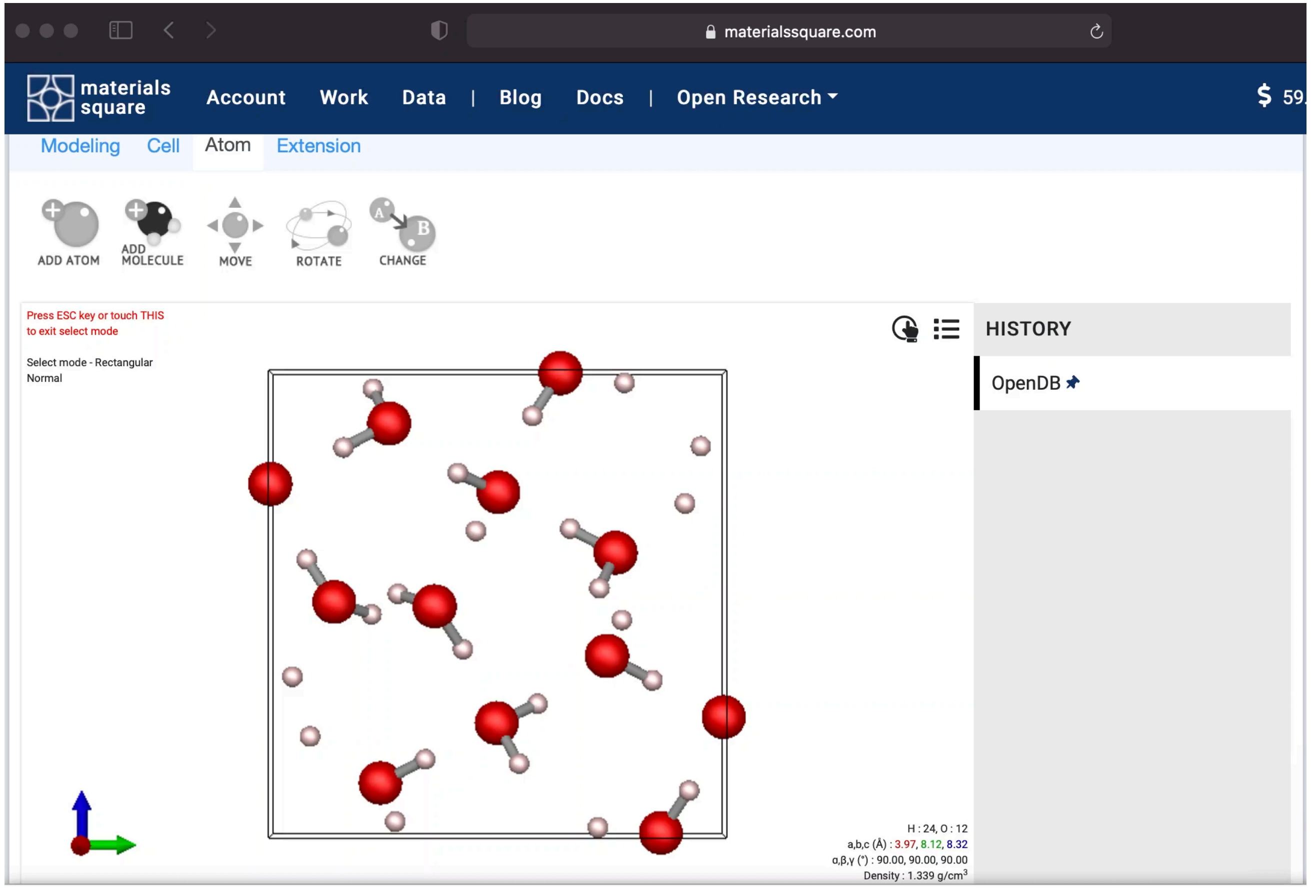
Edit



Materials Square's edit feature

Cell Edit (supercell, cleve etc.)

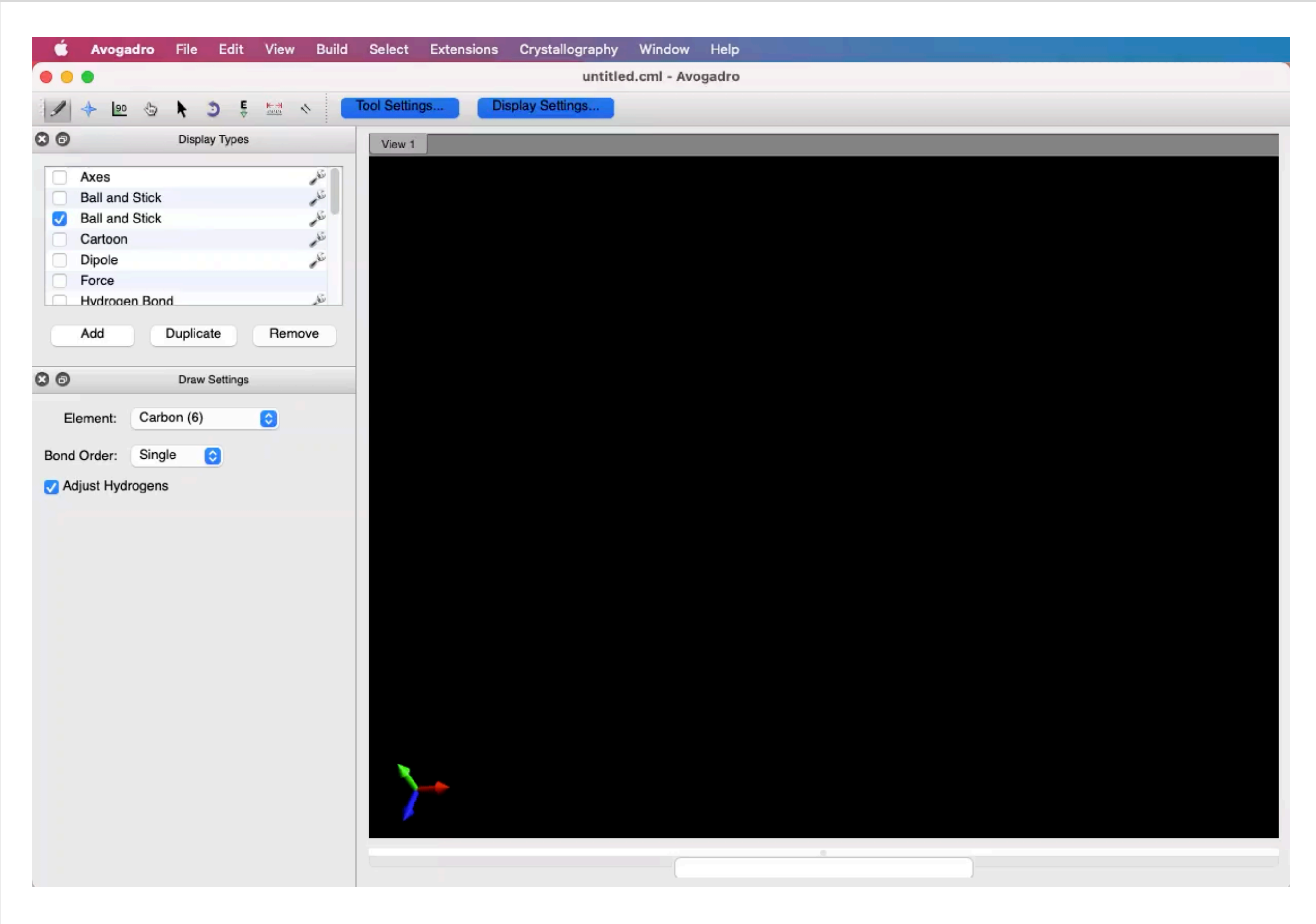
Edit



Materials Square's edit feature

Organic structure builder be scheduled to February.

Edit

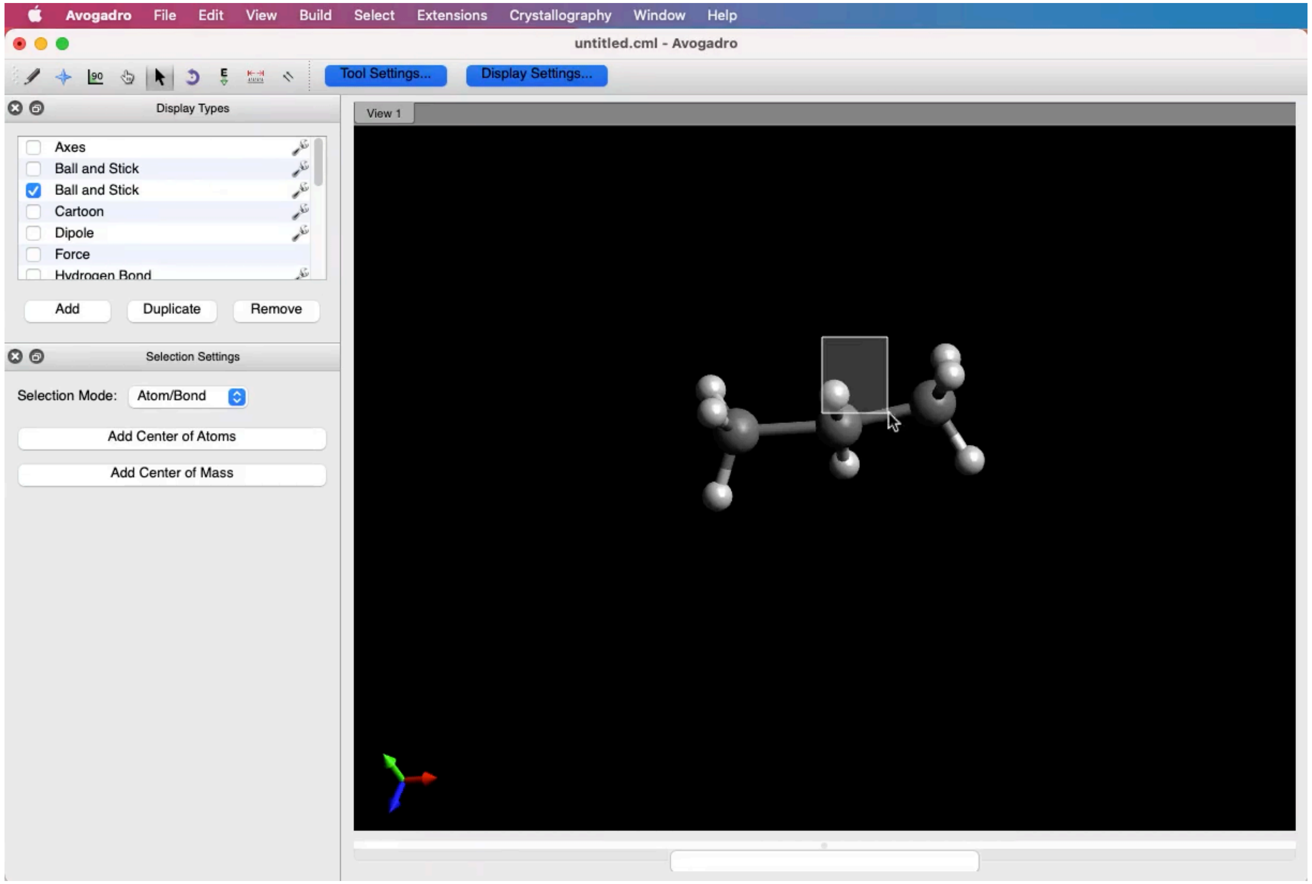


Draw atom

Atom draw using Mouse

Draw with GUI visually easy

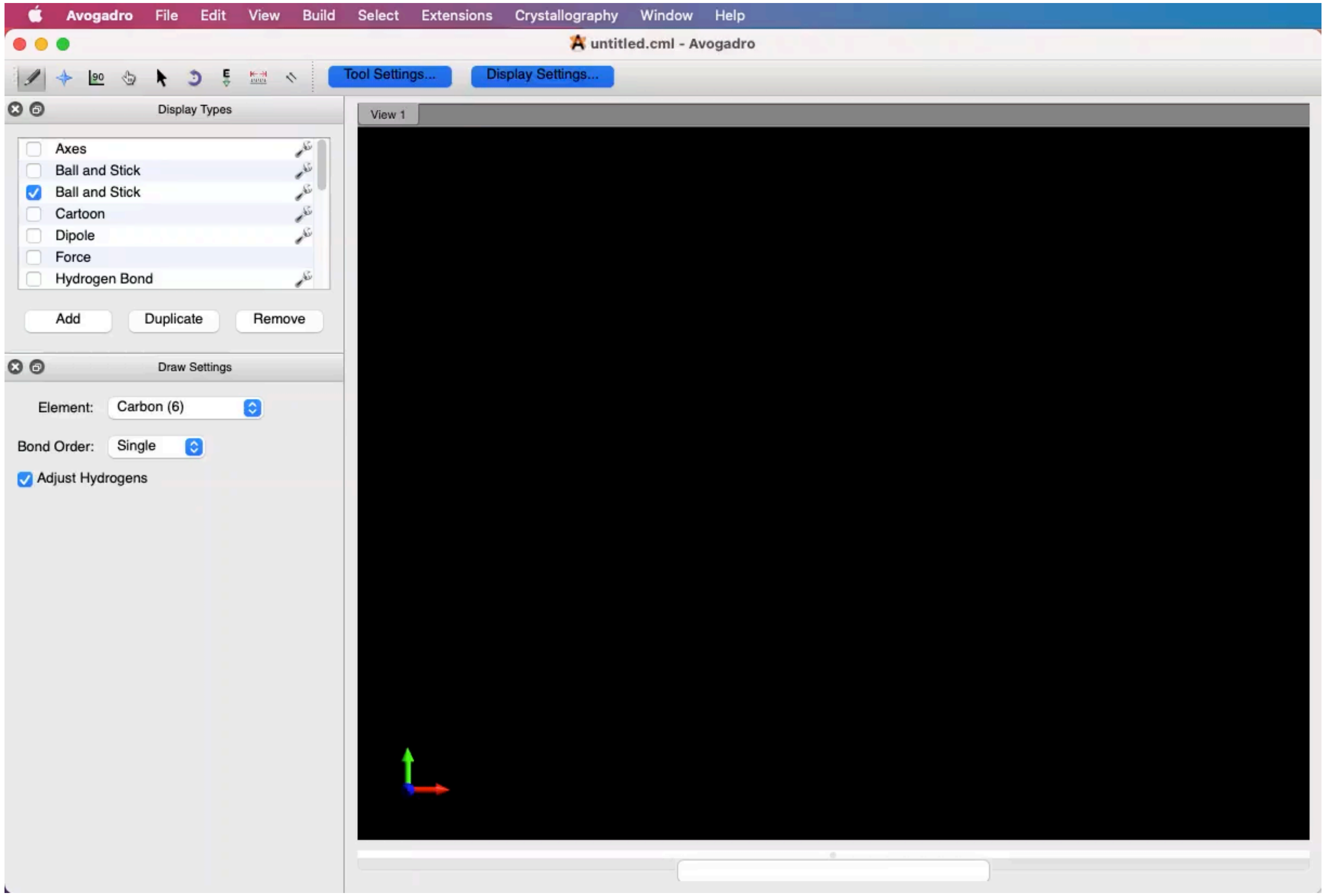
Edit



Manipulate edit

Selected atom edit in detail

Edit



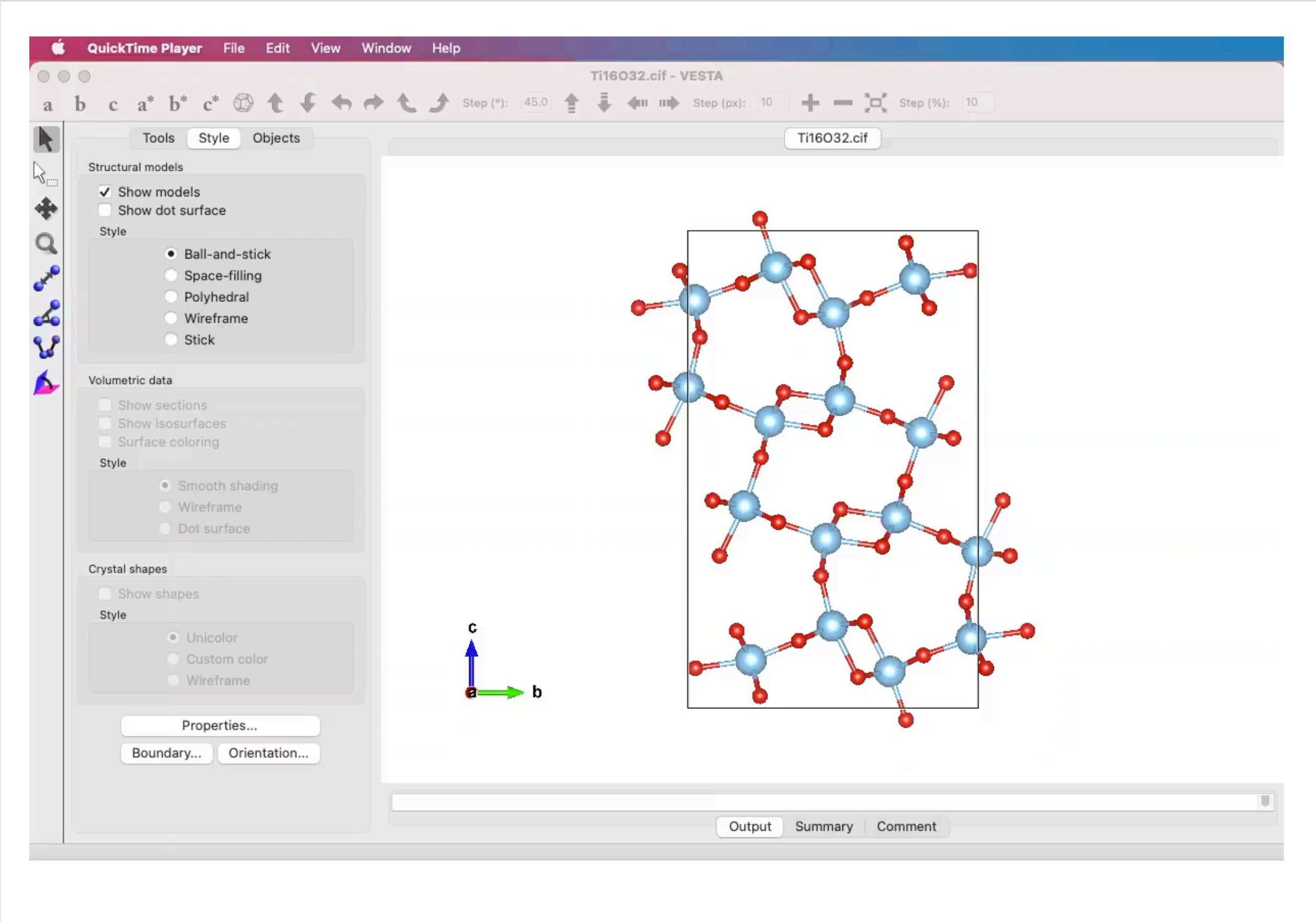
Conformer search

Using inner Forcefield

Roughly drawn structure cleaning

Searching isomer

Edit



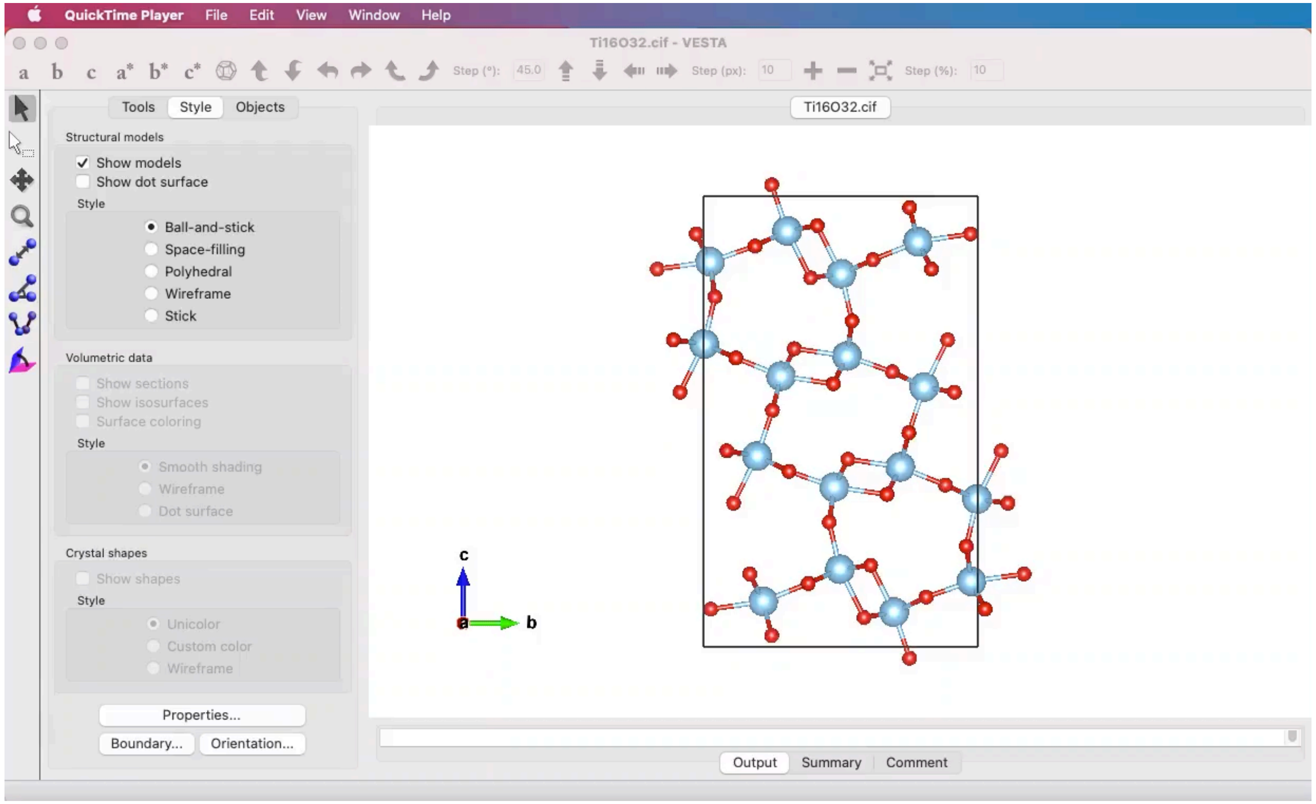
Cell transformation

Characterized to inorganic material

Cell transformation

Use manually

Edit



Data export

Structure file convert to POSCAR

Calculation Input

2 Structure visualizer

- Visibility
- Edit
- **Analysis**
- Performance

Electronic structure

- Density of States
- Charge density
- Band structure
- Orbital surface
- …

Atomic structure

- RDF
- Defects
- Dislocation analysis
- Voronoi analysis
- …

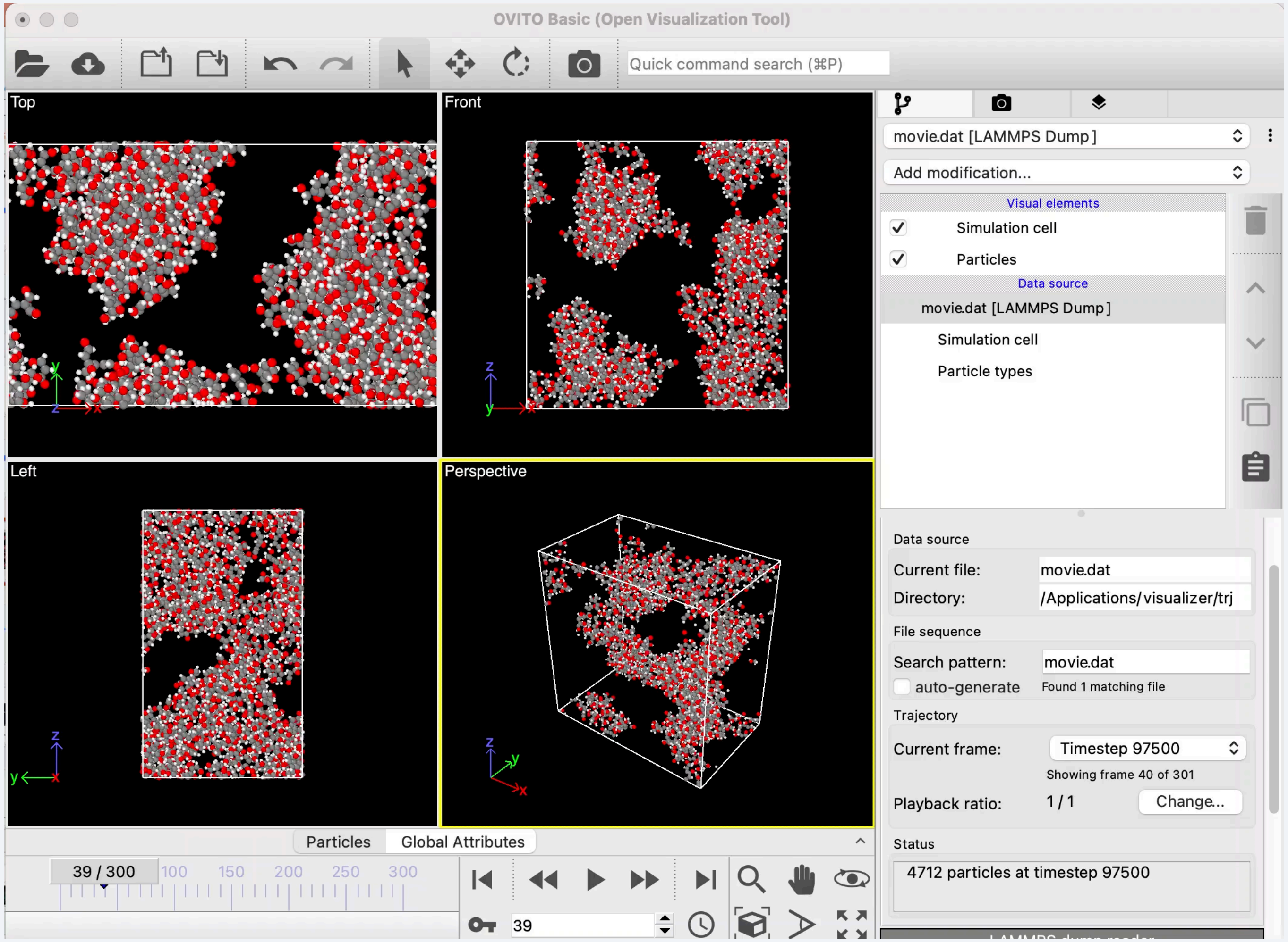
Energetics

- Total Energy
- Binding Energy
- Gibbs Free Energy
- …

RDF

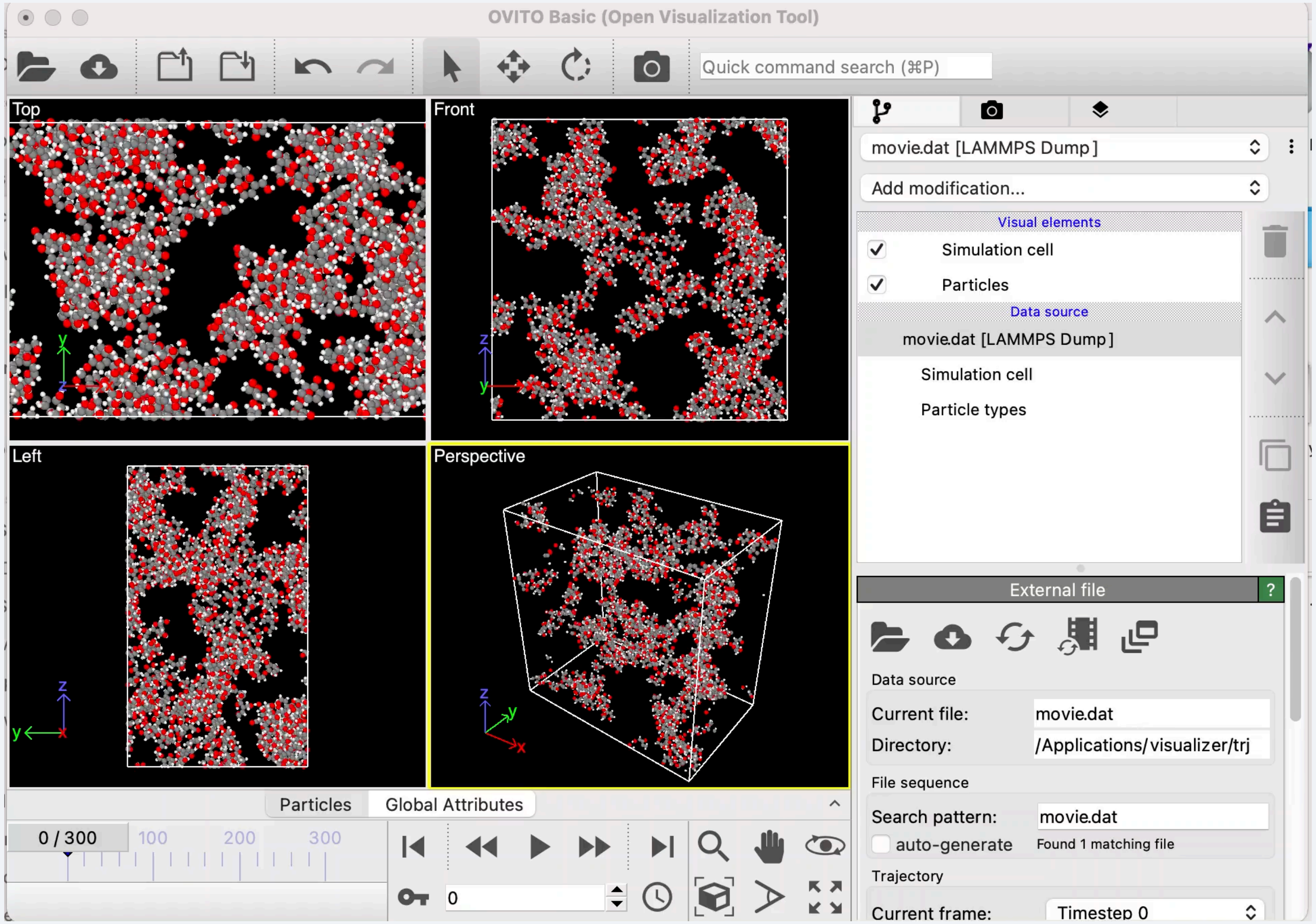
Analysis radial distribution

function



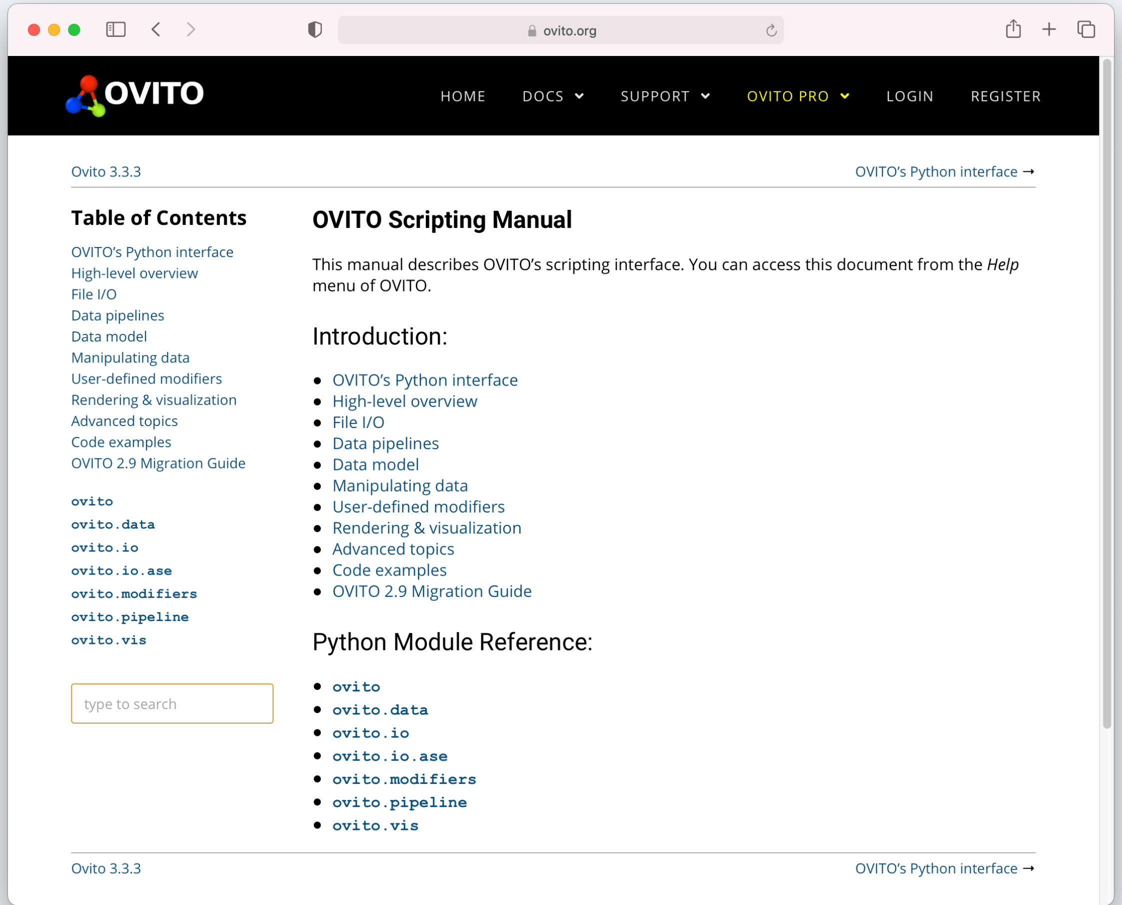
Cluster analysis

Analysis how many cluster in system



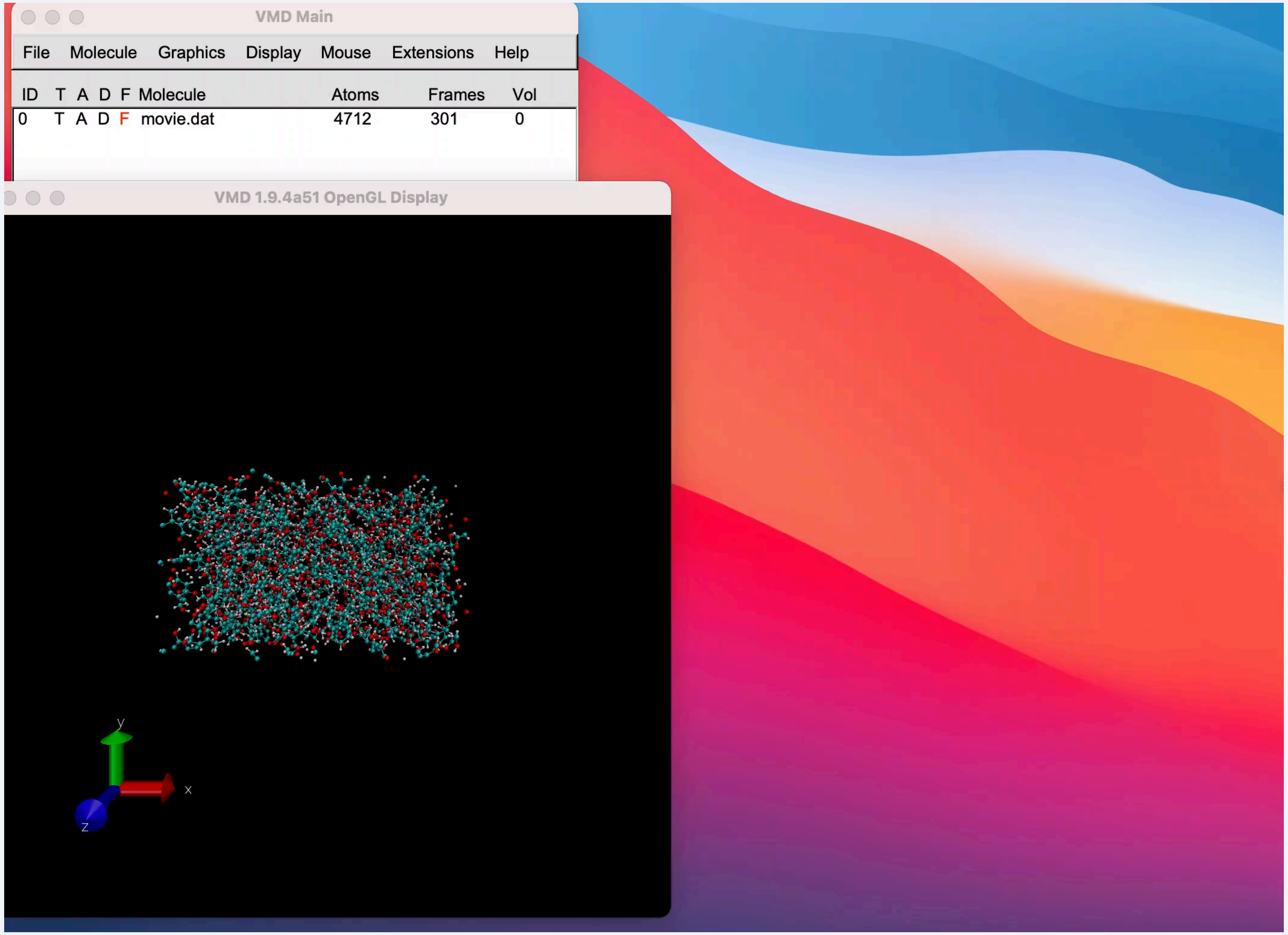
OVITO (Python interface)

- 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.



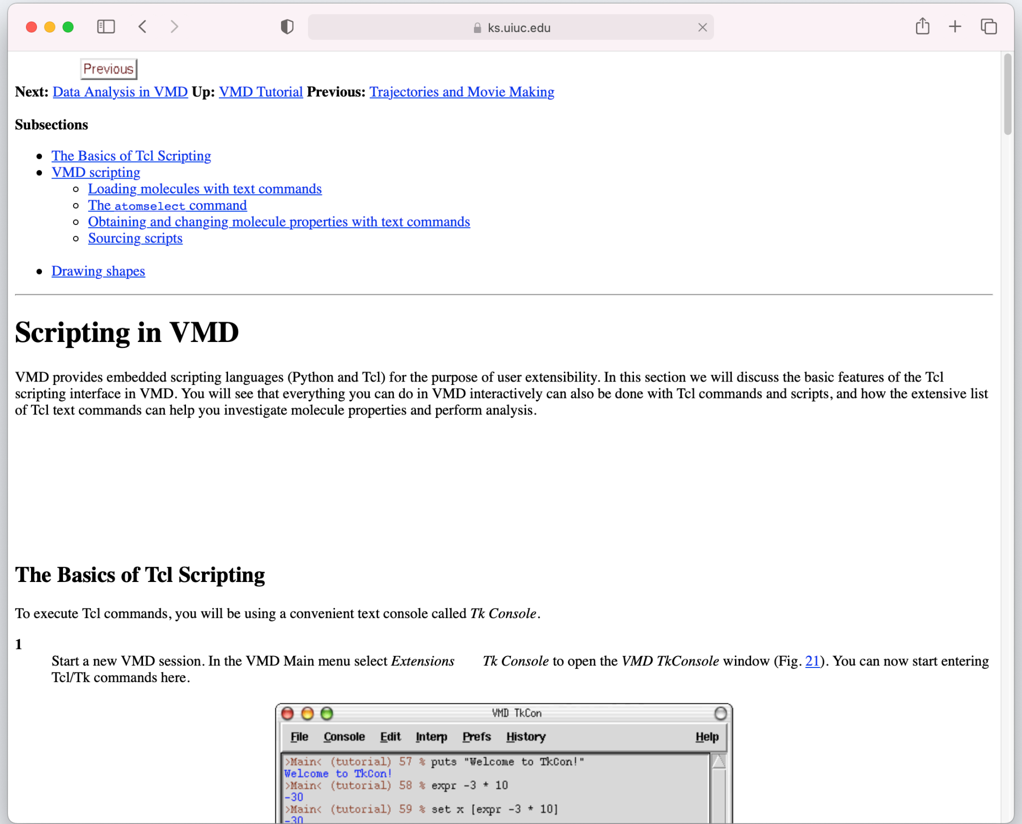
RDF

Analysis radial distribution function



VMD (Tk console)

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

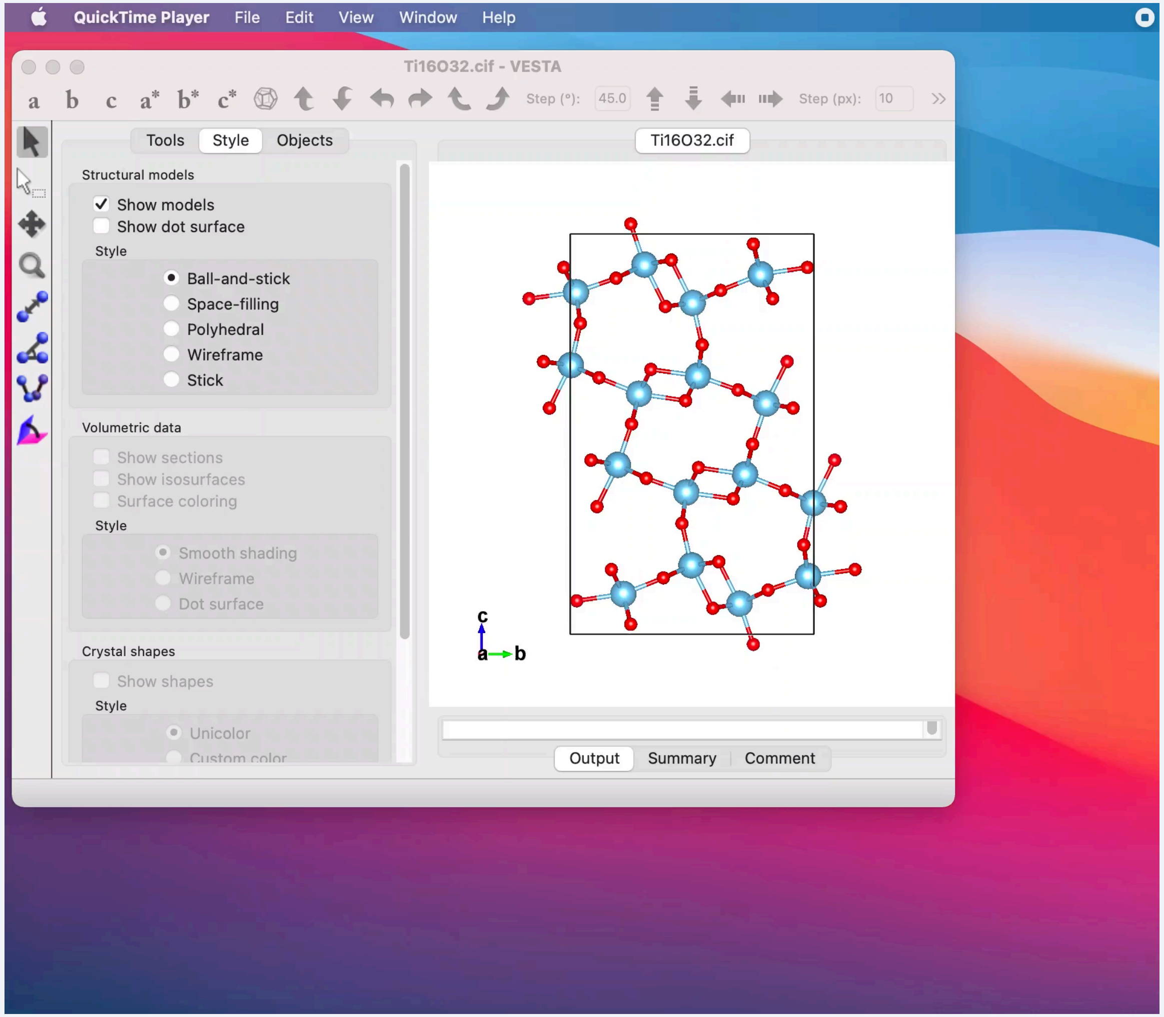


VESTA (XRD pattern)

XRD pattern

Set source wavelength

Crystal information



2 Structure visualizer

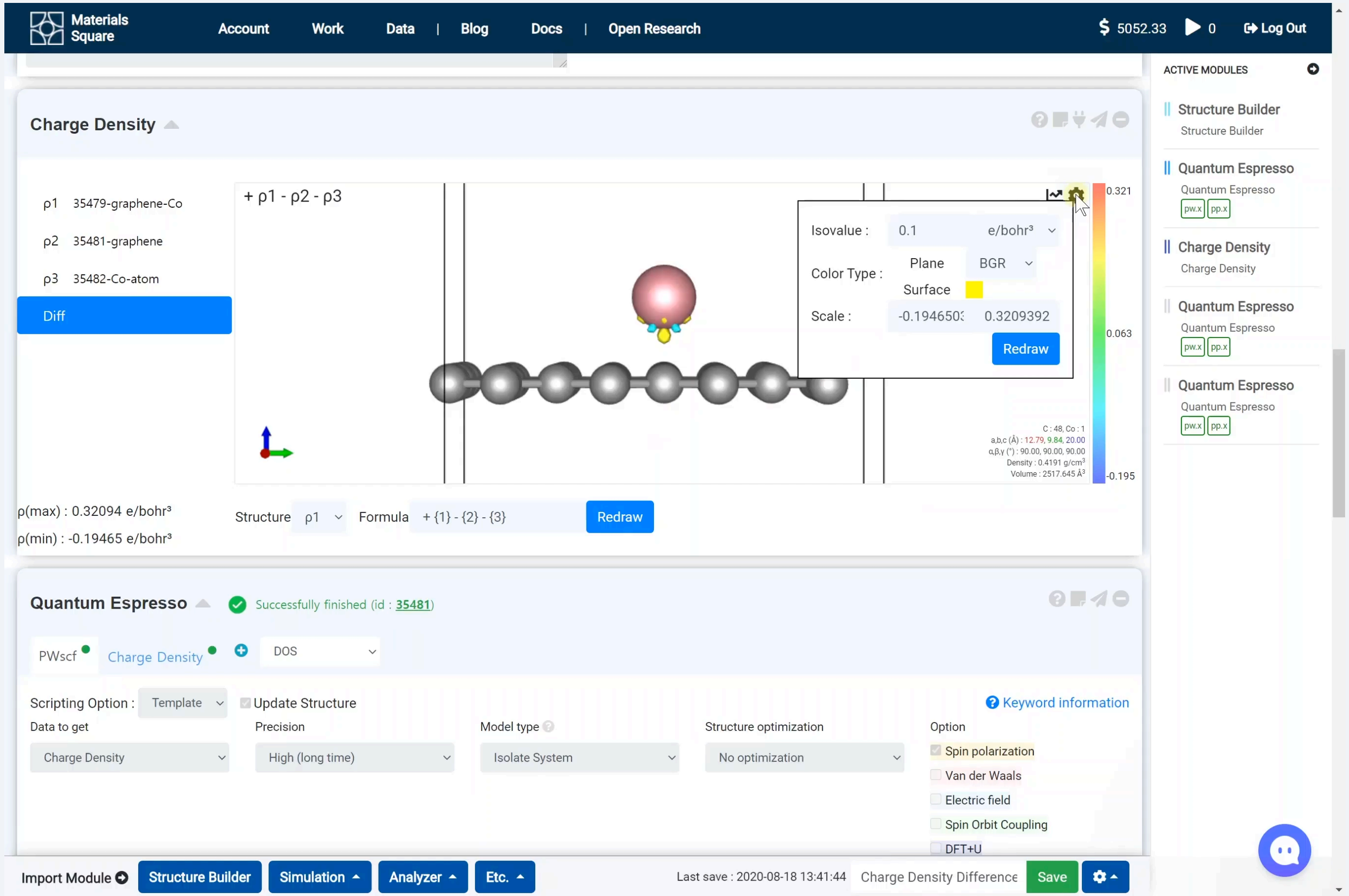
Analysis

MatSQ (Charge Density)

Charge density observe

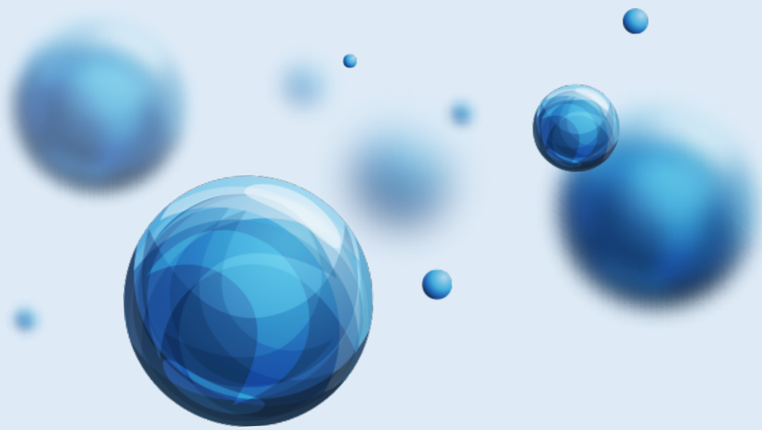
MatSQ (Simulated STM)

Simulated STM image observe



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

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

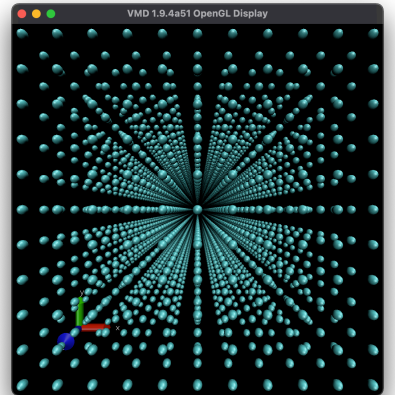
Prepare test structure set

<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