

Building a digital ecosystem for materials R&D including STEM with Mat3ra.com

MAT3RA



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2025.5.22 @ UTK via Zoom

Agenda

The digital ecosystem for Materials R&D

- Brief Introduction: The Company and its Product
- Generic use cases: accelerating the adoption of Modeling & Simulations for electronic materials: interfaces, heterostructures, layered compounds
- Specific use cases @ STEM
- Future outlook
- Q&A

Summary

Mat3ra 4 STEM: accelerating materials R&D for nanoscale

- Advances in nanoelectronics depend on materials, processing, and manufacturing from nanoscale. Mat3ra.com aims to accelerate materials R&D for nanoelectronics by making advanced simulations and AI/ML **accessible & collaborative**.
- Mat3ra:(1) makes adopting Modeling and Simulations (DFT, e.g. MD) and AI/ML tools (Deep Learning forcefields) faster and easier to deploy and use even for non-experts;(2) enables **collaboration** online at intra- or inter-organizational levels increasing productivity and efficiency.
- Mat3ra.com started working on integrating and organizing experimental data, and a set of representative use cases for it. Further development including UTK STEM use cases for nano-electronics are underway.

The Presenter

Pioneering the field of collaborative Digital Materials R&D since 2015



Timur Bazhirov, Ph.D. 

Founder / CEO - Mat3ra.com (prev. Exabyte.io)

Verified email at mat3ra.com - [Homepage](#)

Software-driven materials ...

Cited by	All	Since 2018
Citations	480	253
h-index	13	9
i10-index	15	9

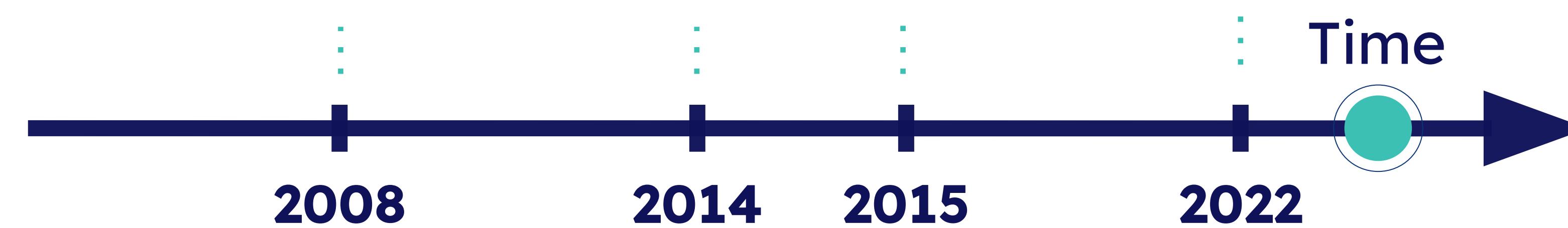
The screenshot shows a news article from The Wall Street Journal. The headline reads "Startup That Models Materials at Atomic Level Raises Seed Capital". Below the headline, there is a section titled "CIO JOURNAL" with the sub-section "MATERIAL". It features a visualization of a molecular structure with atoms labeled with values like 7.7348, 99.2000, 13.758, and 10.2000. To the right, there is a sidebar with the Deloitte logo and several other news snippets.

B.S./M.S. Physics
Moscow Inst. of
Physics & Tech.

Ph.D. Physics at
UC Berkeley,
w/ M. L. Cohen

Started **Exabyte.io**,
to give better modeling
tools to scientists

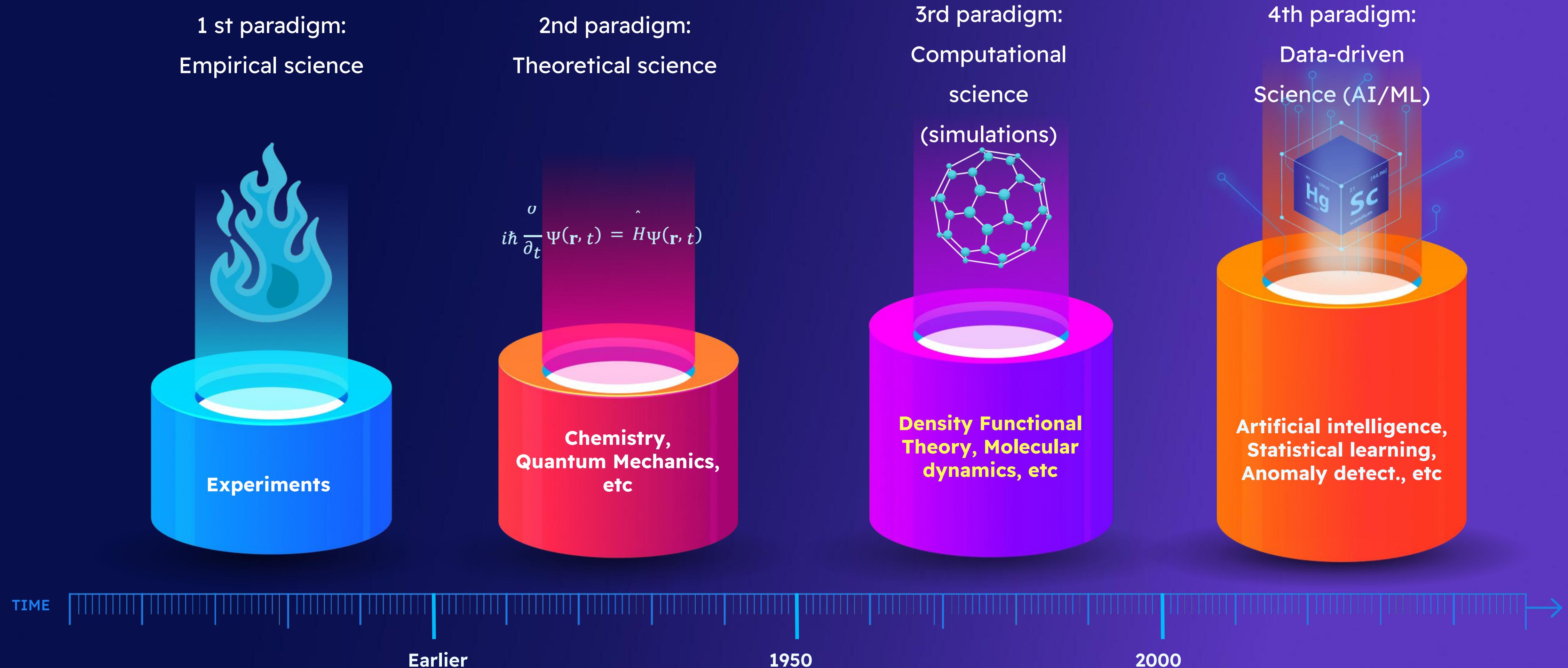
Mat3ra.com emerged
as a successor
of Exabyte.io



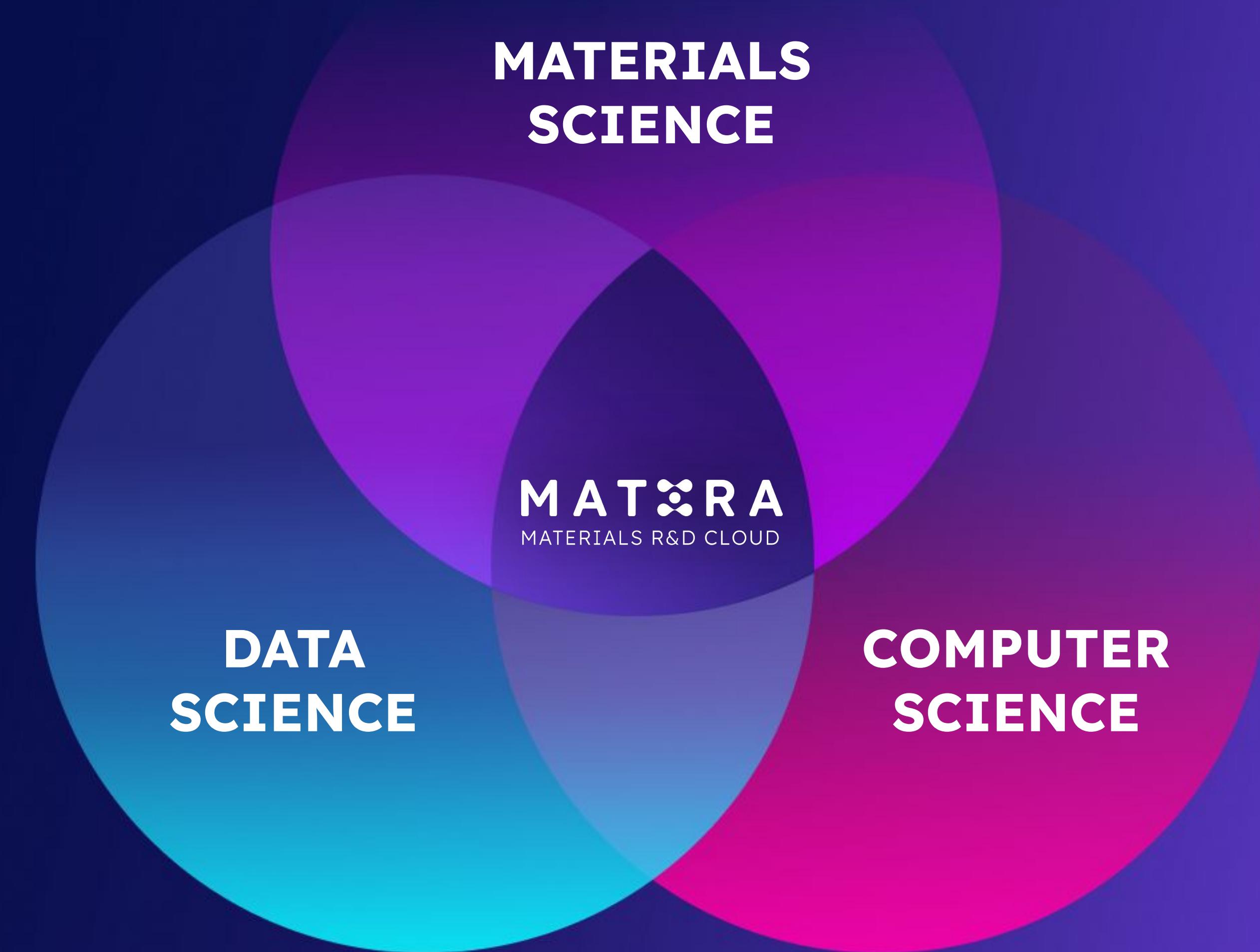
INTRODUCTION

MAT3RA (PRONOUNCED “MA-TEH-RA”):
THE ERA OF DIGITAL MATERIALS R&D
(HENCE THE DIGIT “3” INSTEAD OF “E”)

The 4th Paradigm of R&D: AI/ML



The Circles of AI/ML-driven R&D



Materials R&D Cloud

ANY(!)

COMPUTATIONAL
SCIENTISTS



DATA
SCIENTISTS



EXPERIMENTAL
SCIENTISTS



SECURE



R&D
MANAGEMENT

MULTI-SCALE TOOLS



IT ADMIN

MACHINE
LEARNING

Growing Momentum

Scientists and Engineers around the world use Mat3ra to:



CATALYZE RESEARCH

Accelerate R&D with an easy to use, collaborative & data-centric simulation platform



OPTIMIZE ROI

Optimize productivity through our purpose-built easy-to-use, and highly customizable interface



REFINE SYNERGY

Empower cross-discipline R&D teams with centralized and well-organized data

75,000+

CALCULATIONS
RUN

50,000+

MATERIALS
STORED

25,000+

SCIENTISTS
WORLDWIDE

500+

UNIVERSITIES

25+

ENTERPRISE
CUSTOMERS

Enabling state-of-the-art commercialization for community

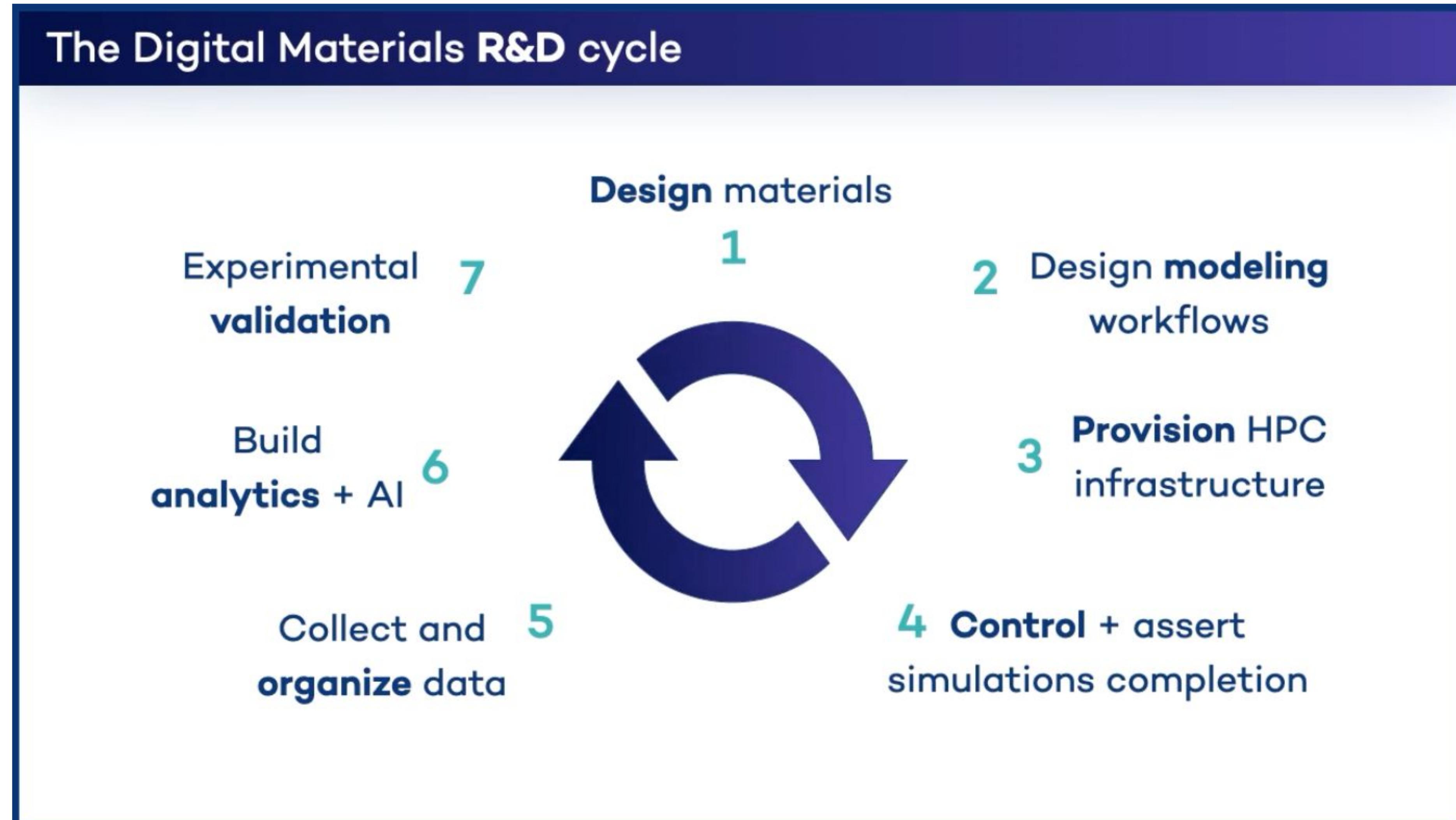
To promote community-wide collaboration and provide an avenue for commercialization



THE MAT3RA PLATFORM

Collaborative end-to-end platform for digital R&D

AI-ready, well-organized structured data. Support for multiple R&D activities. Agile digital practices.



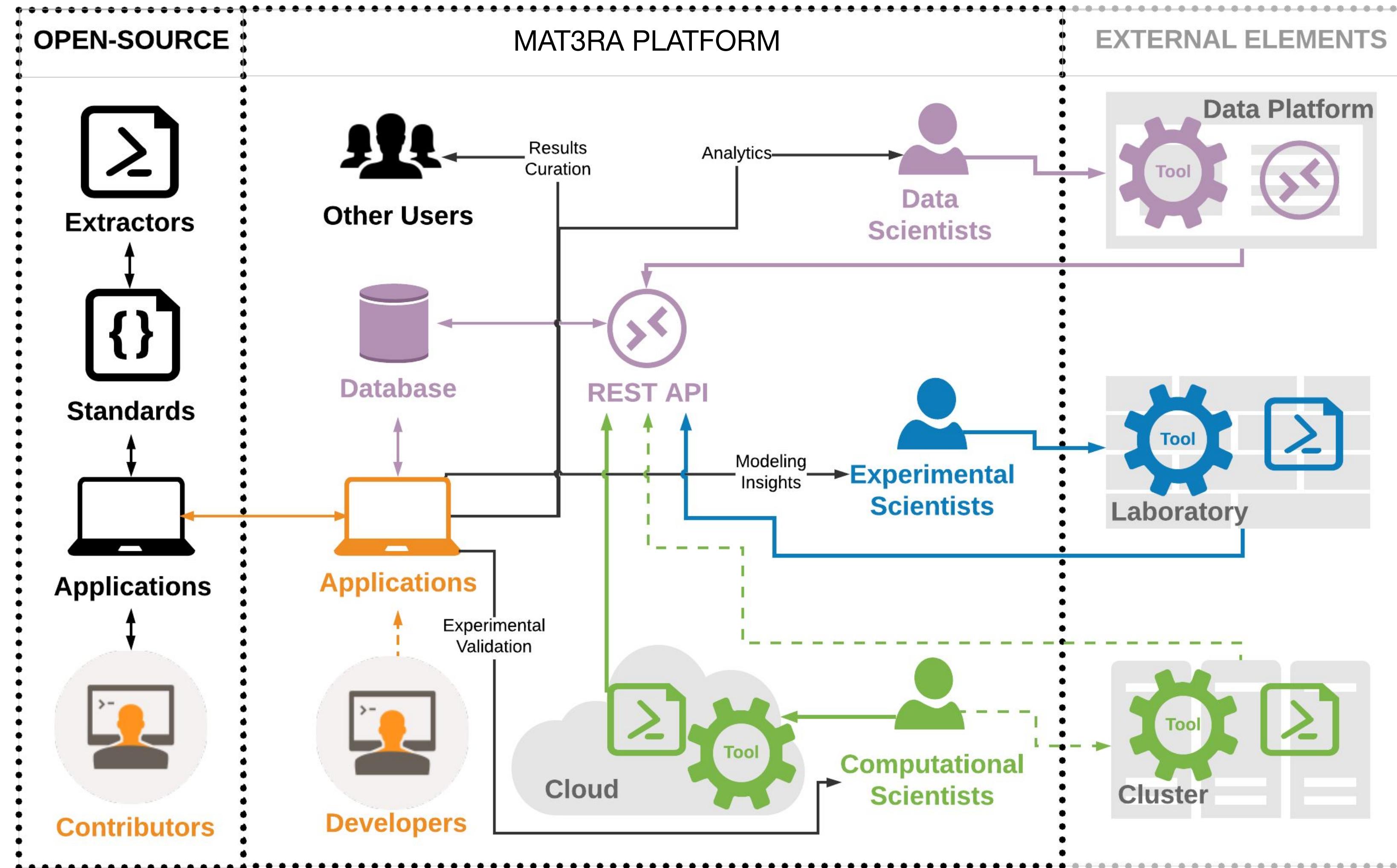
MAT[∞]RA
MATERIALS R&D CLOUD

THE APPROACH

OPEN-SOURCE, MULTI-MODAL

Our approach to organizing Materials R&D

(1) Open-source code, (2) community-driven data, (3) inclusive design for new apps/compute/data



- A comprehensive and flexible approach enabling FAIR (Findable, Accessible, Interoperable, Reusable) data and workflows
- Designed to allow community contributions to reflect the complexity of materials R&D

Our approach to organizing Materials R&D

(1) Open-source codebase and (2) encouraged community contributions

The screenshot shows the GitHub organization page for Mat3ra.com. The top navigation bar includes the GitHub logo, a search bar, and links for Pull requests, Issues, Trending, and Explore. The organization profile card for Mat3ra.com displays a verified badge, 34 followers, location in San Francisco, CA, USA, and contact information via website, Twitter (@mat3ra_com), and email (info@mat3ra.com). Below the profile card, there are tabs for Repositories (68), Packages, People (6), Teams (11), Projects, and Settings. The 'Repositories' tab is selected. The main area is titled 'Pinned repositories' and contains six repository cards:

- esse**: JSON schemas and examples representing structural data, characteristic properties, modeling workflows and related data about materials standardizing the diverse landscape of information. (Python, 1 star)
- express**: ExPrESS: Exabyte Property Extractor, Sourcer, Serializer. A python package allowing to extract and standardize materials data from native format for physics-based simulation engines. (Python, 1 star)
- exabyte-api-examples**: Example usage of Exabyte.io platform through its RESTful API: programmatically create materials and modeling workflows, execute simulations on the cloud, analyze data and build machine learning models. (1 star)
- made.js**: Materials Design in Javascript (made.js). A JavaScript (Node) library allowing for the creation and manipulation of material structures from atoms up on the web. (JavaScript, 2 stars)
- materials-designer**: A standalone React.js/Redux based web application for the design and visualization of atomistic materials structures. Used within the Exabyte.io platform and can be deployed in standalone mode. (JavaScript, 2 stars)
- exparser**: A python package converting materials modeling (eg. DFT) data on disk to a structured representation according to ESSE and ready for indexing and database storage. (Python)

On the right side of the pinned repositories section, there is a link to 'Customize pinned repositories'.

USE CASES

HOW THE PLATFORM IS USED

Representative Case Studies

Representative case studies demonstrating what's possible today: <https://docs.mat3ra.com/tutorials/overview/>.

1. Semiconductor / Electronic Materials

- Thin-Films, Heterostructures, Schottky Barrier, Band Offset
- Spectroscopic data: IR-Raman spectra

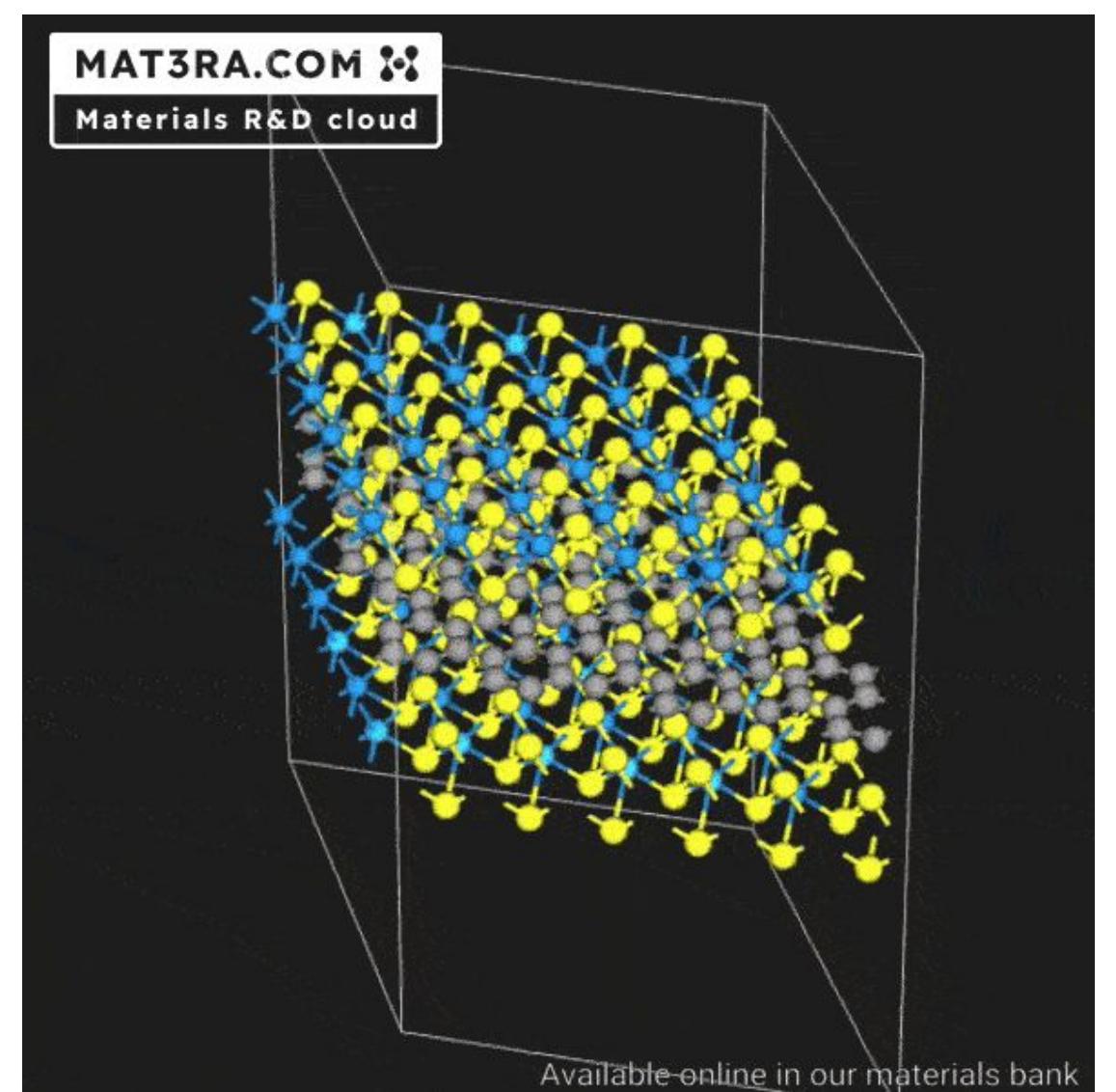
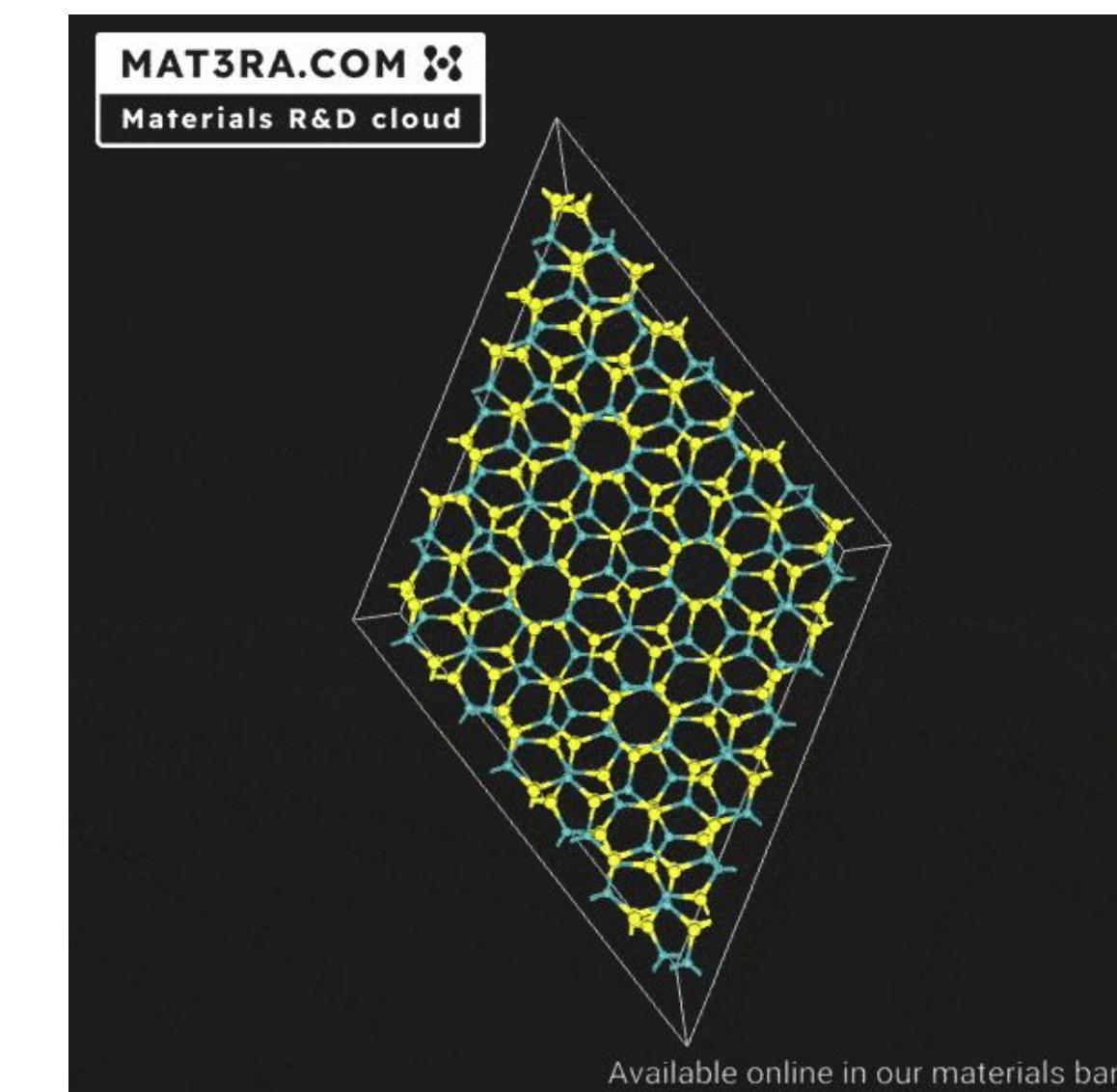
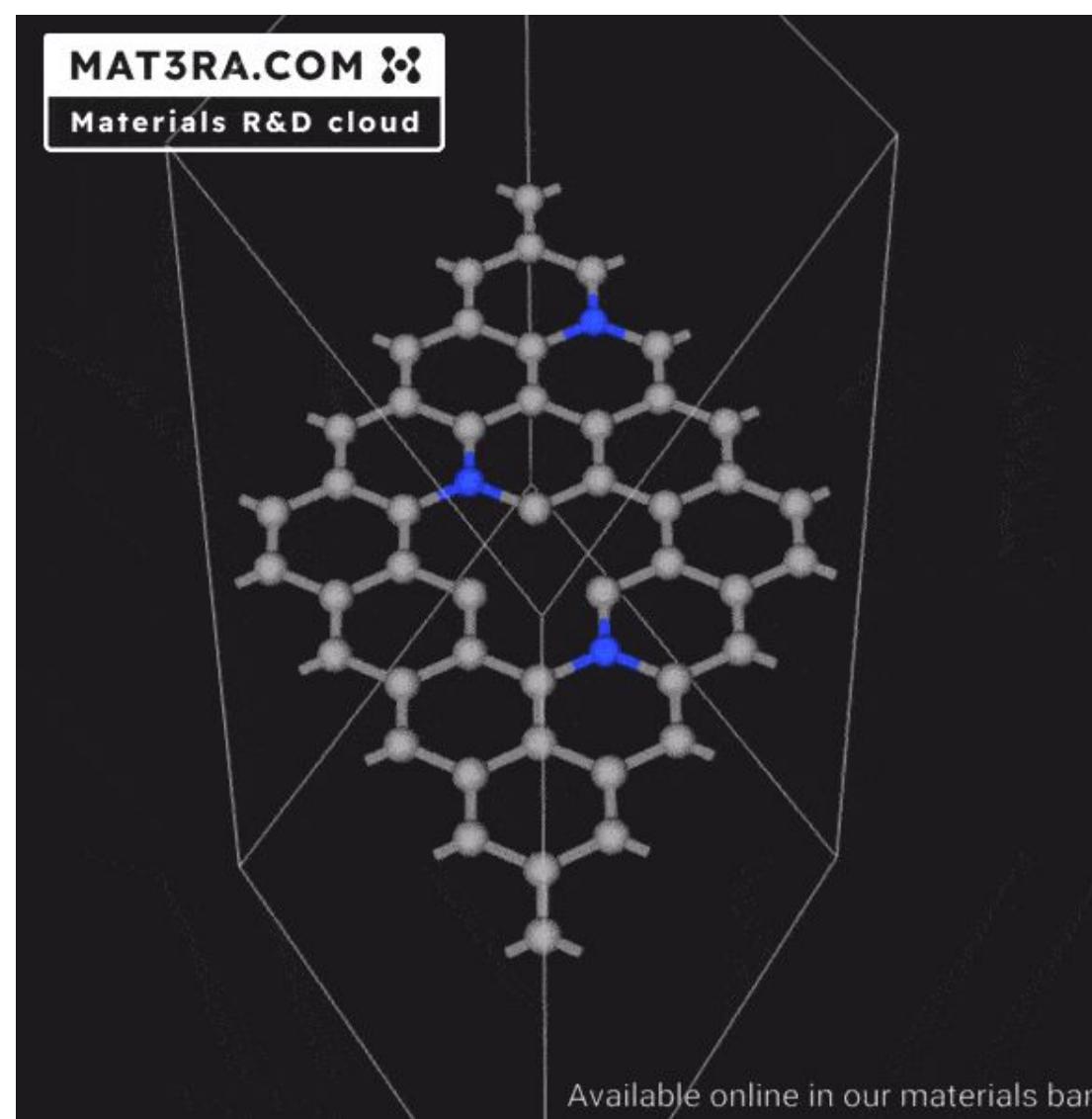
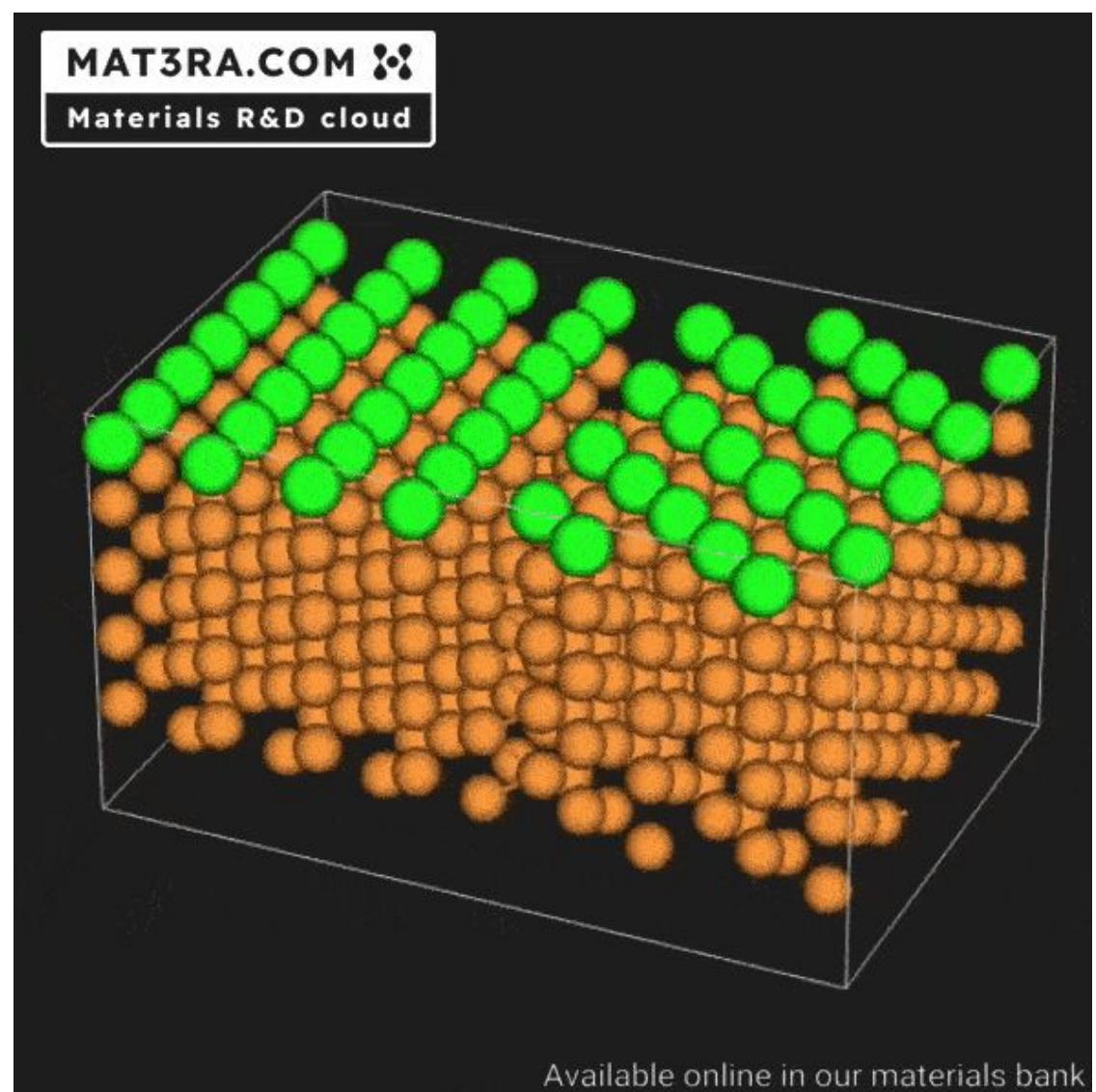
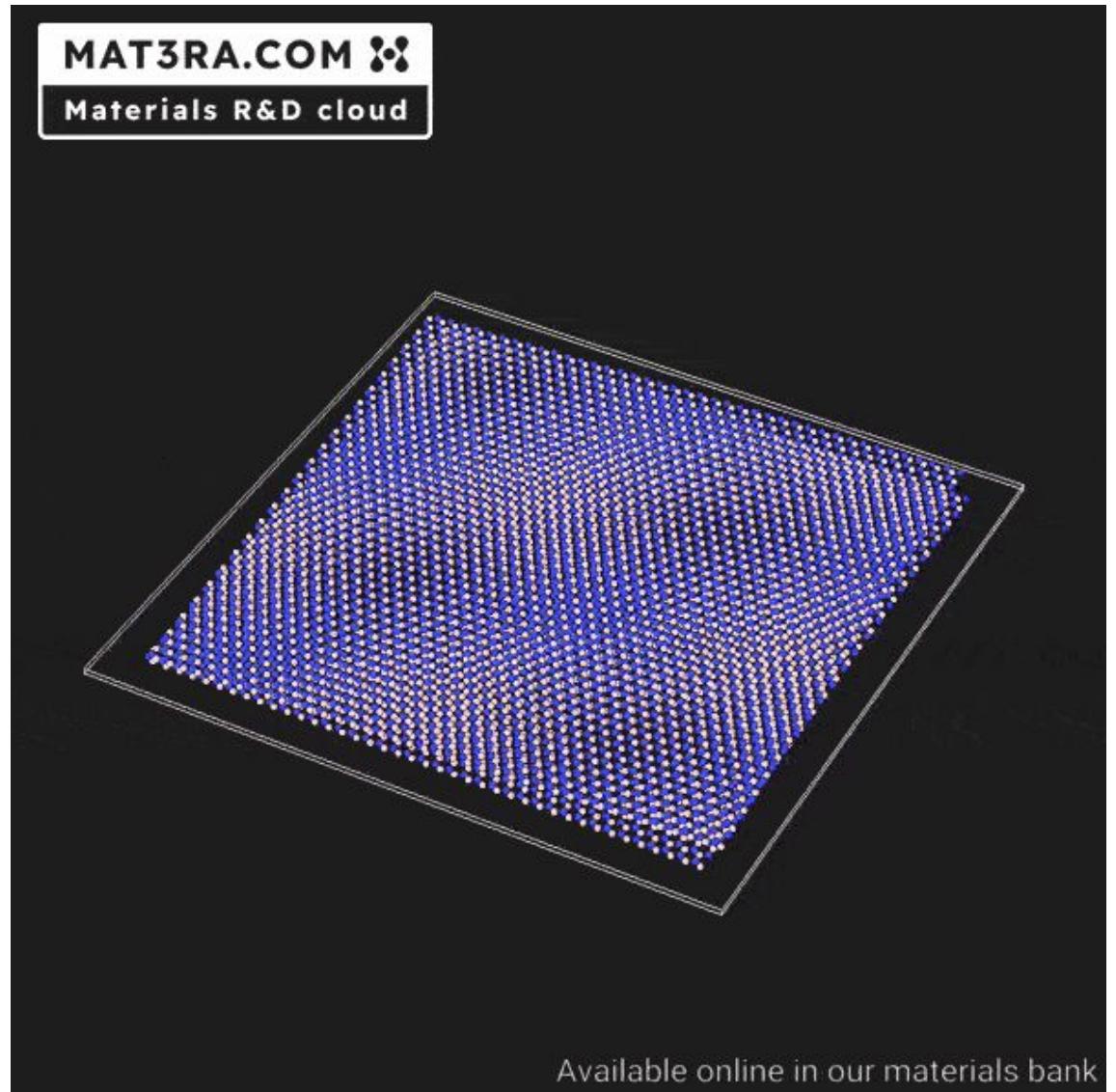
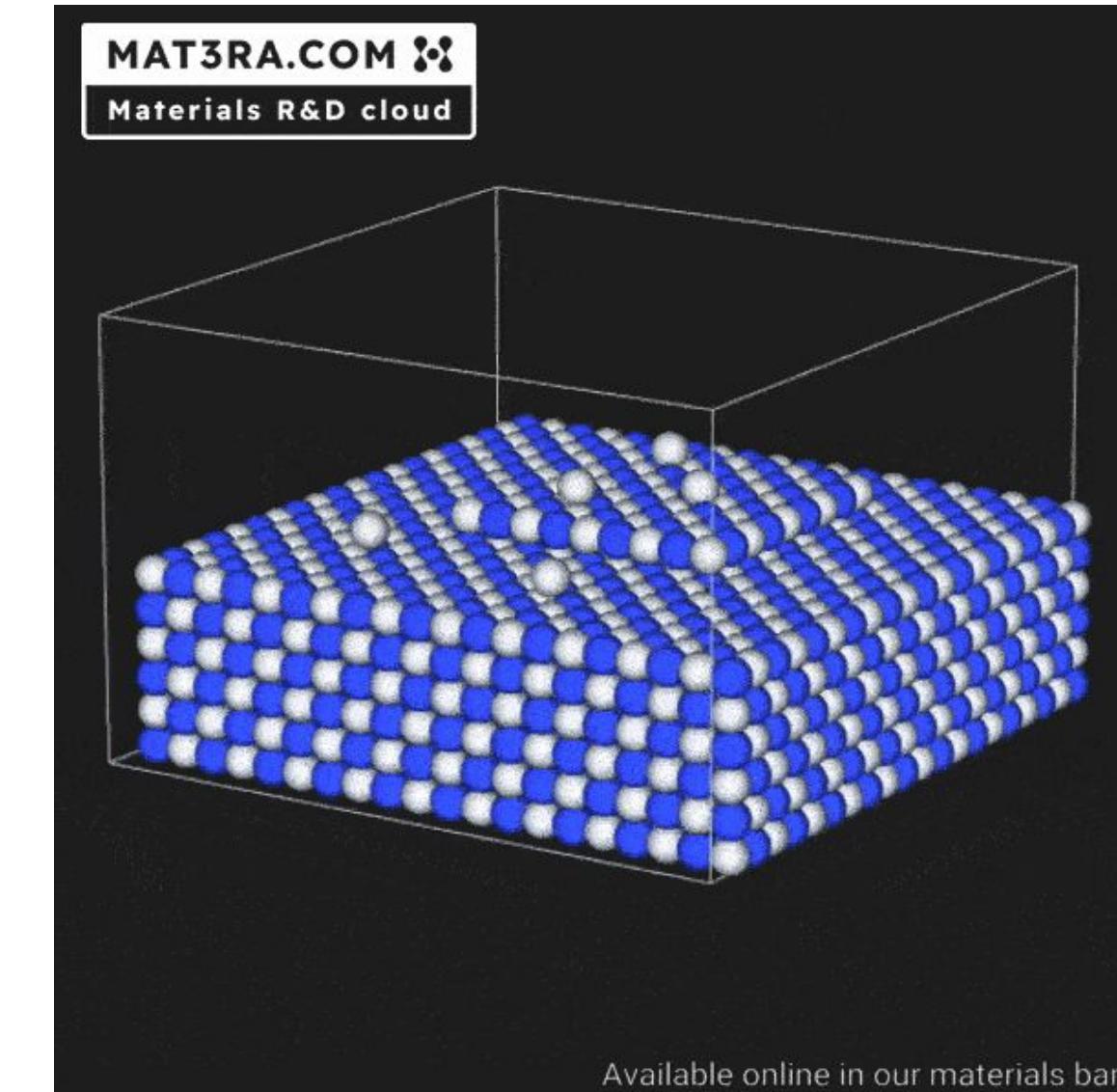
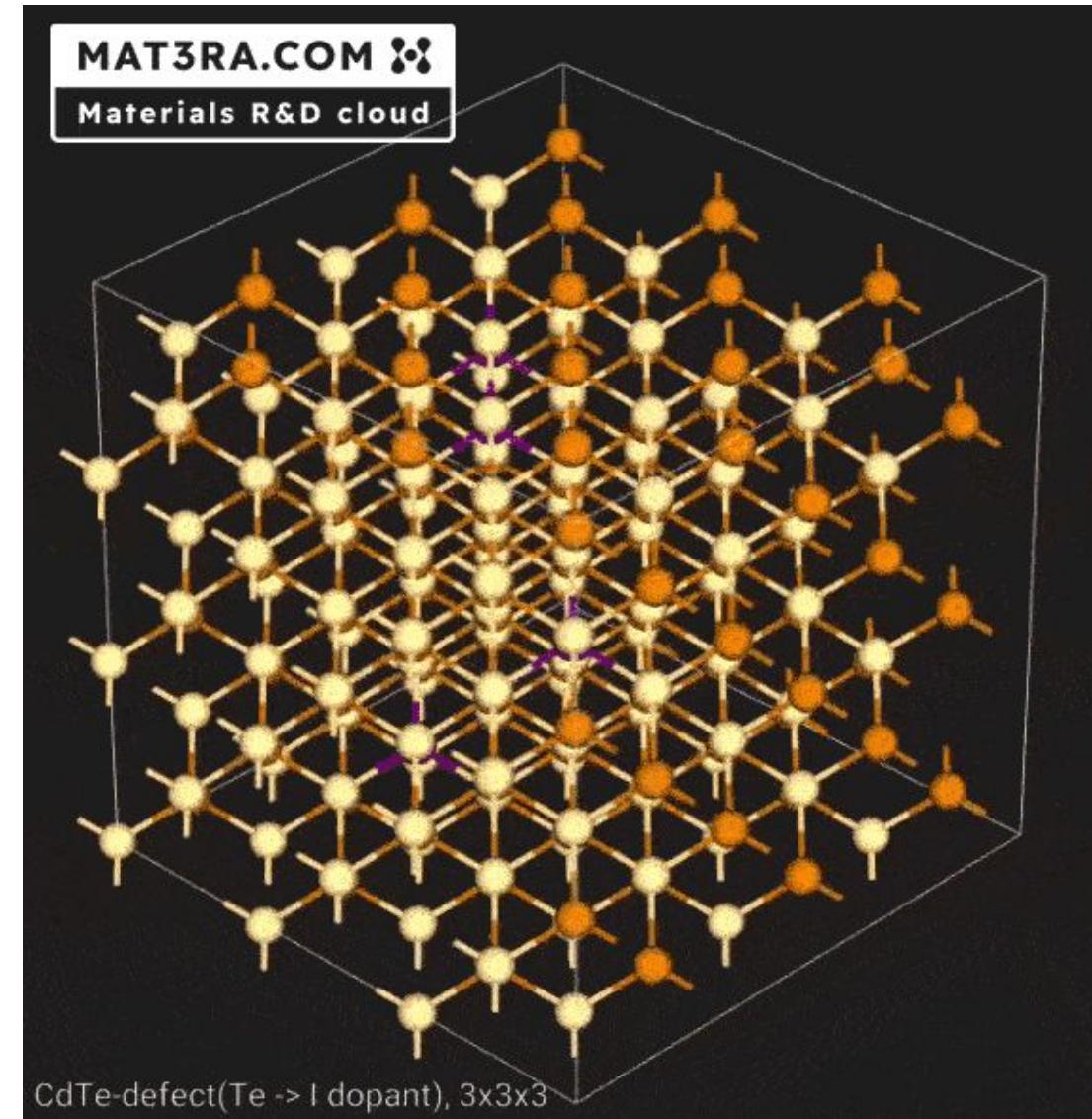
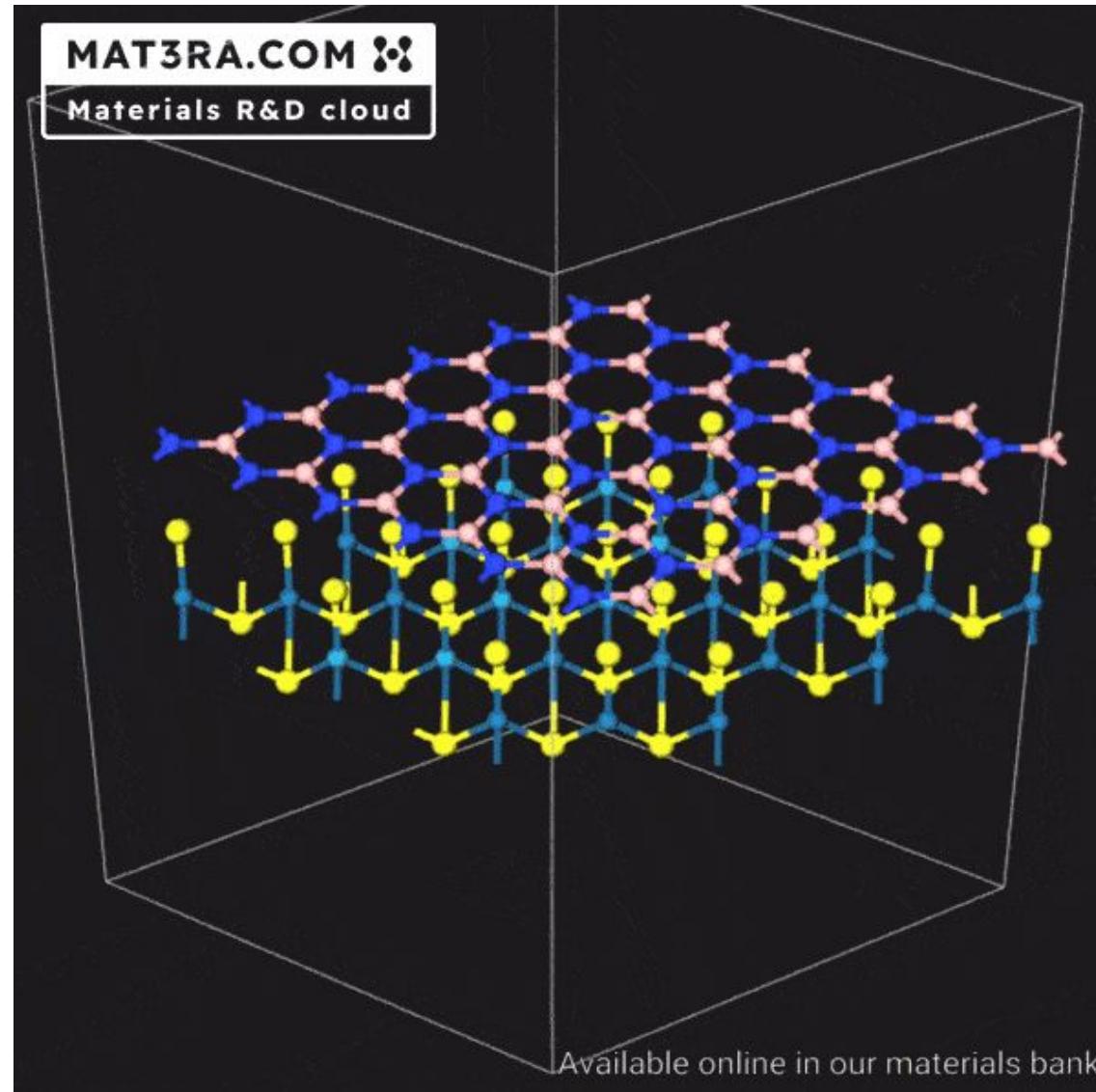
2. Nano-materials - (Proof-of-Concept)

- Thermal Conductivity of Carbon Nanotubes
- Adsorption Energy of metal nanoclusters, Surface energy of layers

3. Polymers / Plastics / Resins - (Proof-of-Concept)

- Metal/Resin, Fiber/Matrix bonding and adhesion strength
- Stress/strain curves for polymer thermoplastics

Design 2D Materials & Heterostructures w/ Defects, disorder



EXAMPLE WORKFLOW: VALENCE BAND OFFSETS

platform.mat3ra.com/timur/materials/PHANQB564yHCQA53A

Timur Bazhirov
Individual

Home > Account > Materials - Heterostructure - JVASP-670 with JVASP-664 - 2024-03-14

Heterostructure - JVASP-670 with JVASP-664 - 2024-03-14
formula Te₆Mo₇S₈ lattice HEX

Lattice
HEX

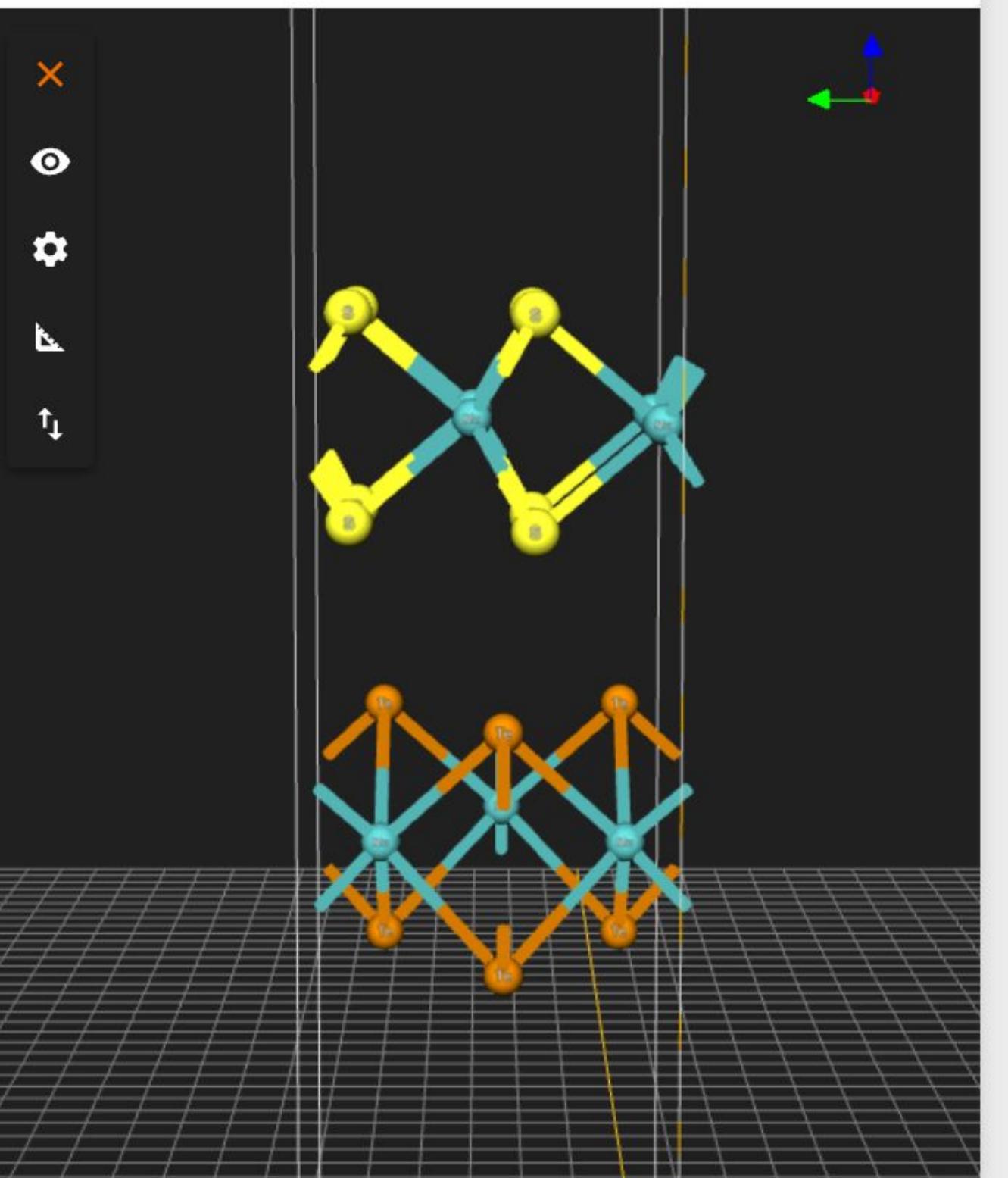
a 6.3759 b 6.3759 c 25.757
α 90.000 β 90.000 γ 60.000

Basis

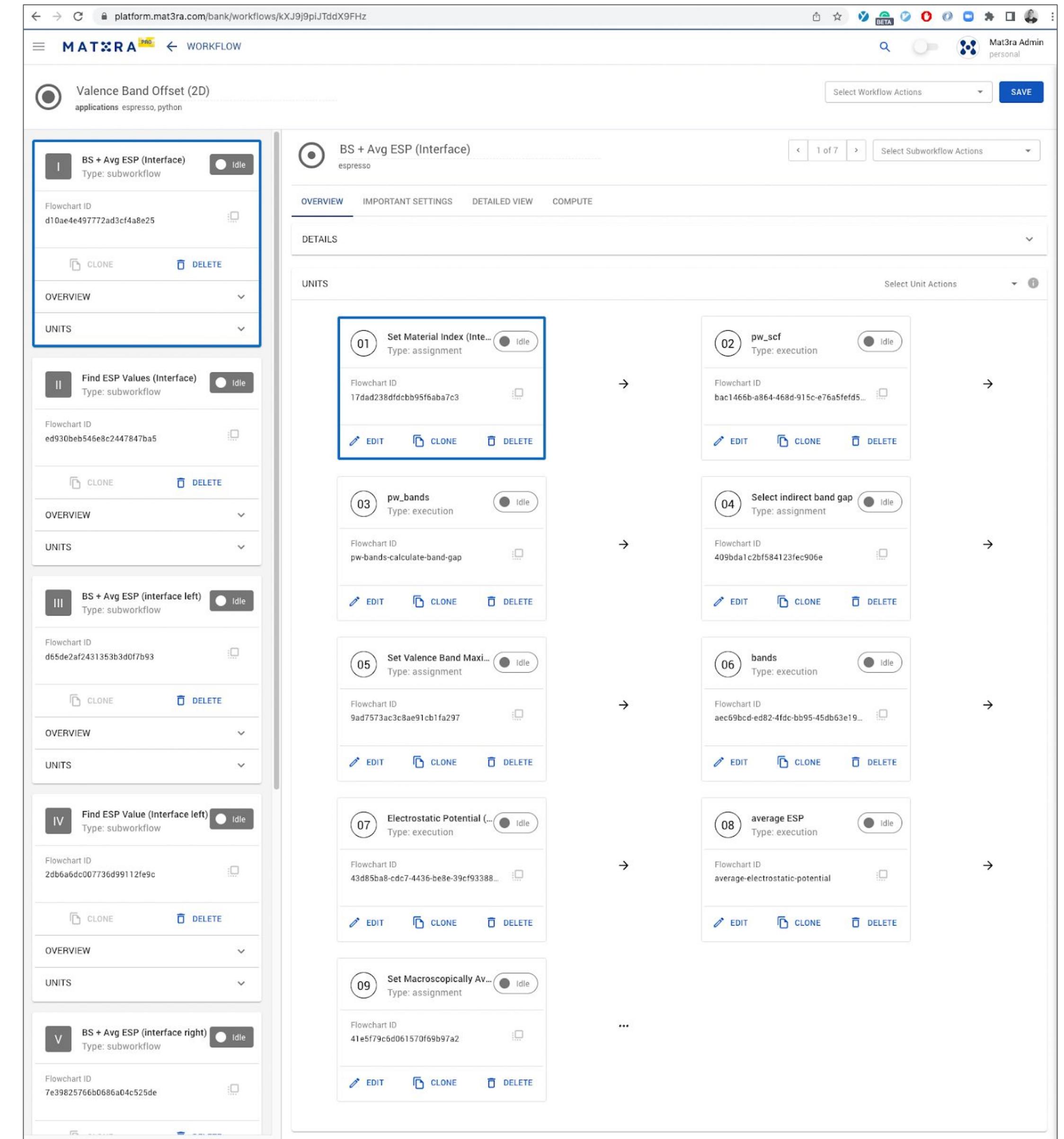
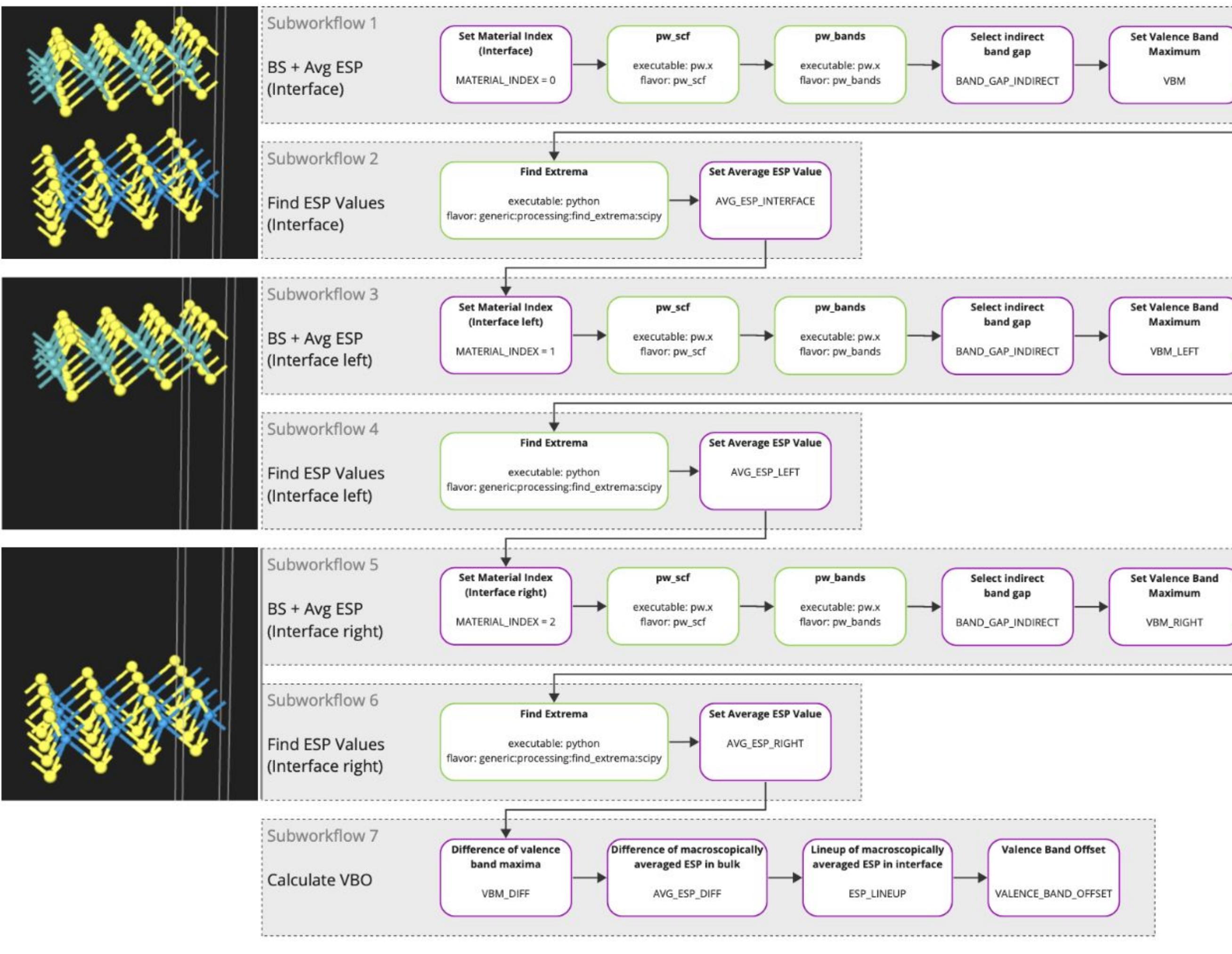
1 Mo	0.361111	0.027777	0.606133
2 Mo	0.555556	0.111111	0.358489
3 Mo	0.222223	0.777777	0.358489
4 Mo	0.888889	0.444444	0.358489
5 Mo	0.361111	0.527777	0.606133
6 Mo	0.861111	0.527777	0.606133
7 Mo	0.861111	0.027777	0.606133
8 S	0.194444	0.361111	0.545311
9 S	0.694444	0.861112	0.666956
10 S	0.694444	0.361111	0.666956
11 S	0.194444	0.361111	0.666956
12 S	0.694444	0.861112	0.545311
13 S	0.694444	0.361111	0.545311
14 S	0.194444	0.861112	0.545311
15 S	0.194444	0.861112	0.666956
16 Te	0.888889	0.111111	0.288139
17 Te	0.555555	0.777778	0.288139
18 Te	0.222222	0.444445	0.428839
19 Te	0.888889	0.111111	0.428839

unit cell volume (Å³) density (g/cm³) space group elemental ratio - Mo elemental ratio - S elemental ratio - Te

906.814 3.101 P1 0.333333 0.380952 0.285714



Valence Band Offset (2D) Workflow





New Job Nov 14, 2022, 18:49 PM

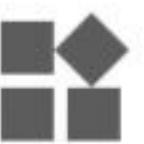
project Default

Select Job Actions

▼

SAVE

1. MATERIALS



Silicon FCC

formula Si lattice FCC

2. WORKFLOW

3. COMPUTE

◀ 1 of 1 ▶

Select Material Actions

▼

Lattice

FCC

a 3.8670

b 3.8670

c 3.8670

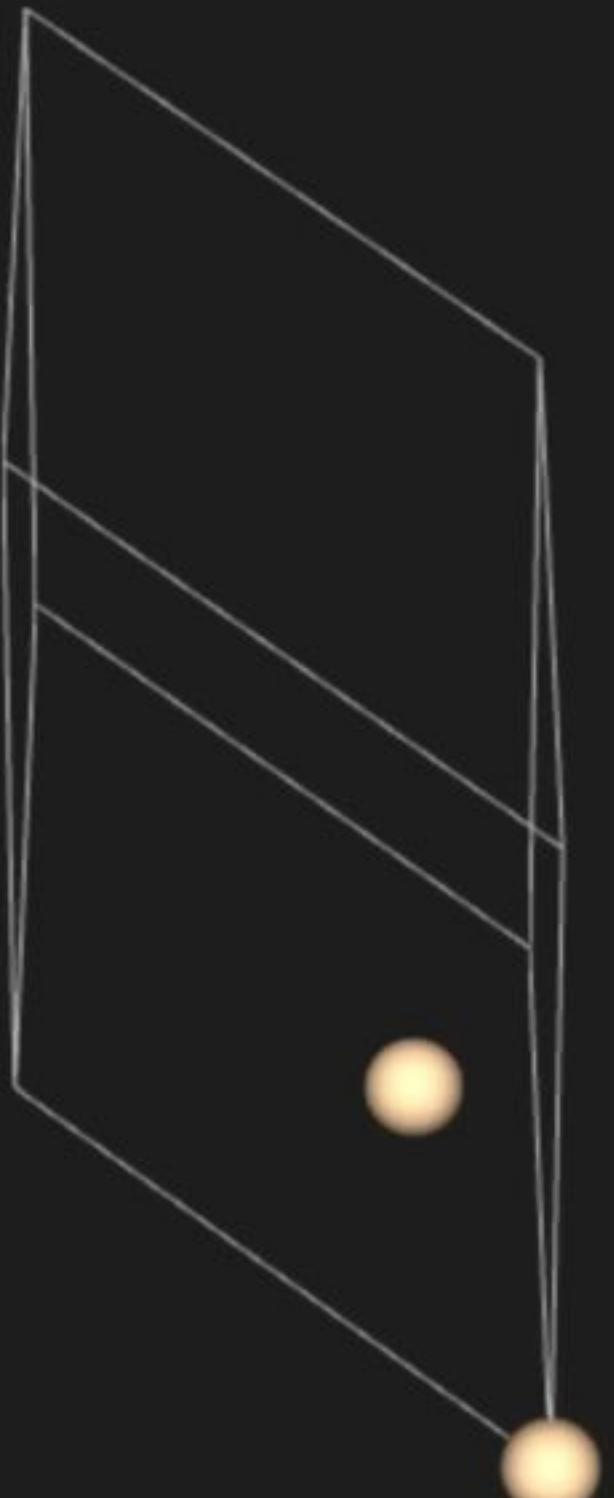
α 60.000

β 60.000

γ 60.000

Basis

1 Si	0.000000	0.000000	0.000000
2 Si	0.250000	0.250000	0.250000
3			



Select Materials (materials collection)

🔍 Click to filter items below ...

1-4 of 4 materials ▾ 1 selected ×



Select Items

	NAME & FORMULA	LATTICE & SYMMETRY	TAGS	NON-PERIODIC	DEFAULT	SHARED	PUBLIC	EXT+LNK	EXT+WEB
<input type="checkbox"/>	WS2 W1 S2	HEX P-6m2				<input checked="" type="checkbox"/>			
<input type="checkbox"/>	MoS2 Mo1 S2	HEX P-6m2				<input checked="" type="checkbox"/>			
<input checked="" type="checkbox"/>	interface_WS2_MoS2 Mo1 W1 S4	HEX P1				<input checked="" type="checkbox"/>			
<input type="checkbox"/>	Silicon FCC Si2	FCC Fd-3m			<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>		

1-4 of 4 materials ▲ 1 selected ×



Select Workflow



valence



1-20 of 42 workflows ▾ 0 selected



NAME	SUBWORKFLOWS	TAGS	DEFAULT	UP-TO-DATE	SHARED	PUBLIC	EXT+LNK	EXT+WEB
<input type="checkbox"/> Valence Band Offset (2D) espresso 5.4.0, python 3.8.6 	<div>BS + AVG ESP (INTERFACE) FIND ESP VALUES (INTERFACE)</div> <div>BS + AVG ESP (INTERFACE LEFT) FIND ESP VALUE (INTERFACE LEFT)</div> <div>BS + AVG ESP (INTERFACE RIGHT) FIND ESP VALUE (INTERFACE RIGHT)</div> <div>CALCULATE VBO</div>							

1-20 of 42 workflows ▲ 0 selected



Unit settings



average ESP

type: execution

description: flowchartId: average-electrostatic-potential-left

Next

Set Macroscopically Averaged ESP Data (82457d05060e984372d45f65)

FlowchartId

82457d05060e984372d45f65

DETAILS

INPUT

AVERAGE.IN

TEMPLATE PREVIEW

UNWRAP LINES

```
1 1
2 pp.dat
3 1.0
4 3000
5 3
6 3.000
```



Flowchart ID

ad8f9d0f1df1836dcbb531de



CLONE

DELETE

OVERVIEW



UNITS



III

BS + Avg ESP (interface left)

Idle

Type: subworkflow

Flowchart ID

8986b86be5e750ced5c01c0b



CLONE

DELETE

OVERVIEW



UNITS



IV

Find ESP Value (Interface left)

Idle

Type: subworkflow

Flowchart ID

77a786f07fade3637b166bb1

**cutoffs**

Planewave cutoff parameters for electronic wavefunctions and density. Units are specific to simulation engine.

wavefunction

40

density

200

Unit 1: pw_scf

kgrid

3D grid with shifts. Default min value for KPPRA (kpt per reciprocal atom) is 10.

dimensions*

6

2

2

shifts*

0

0

0

KPPRA

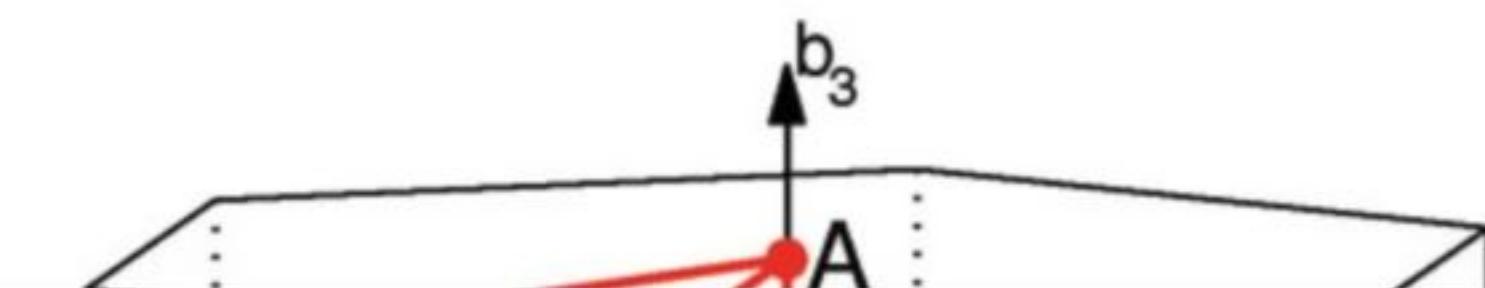
144

 preferKPPRA

Unit 2: pw_bands

kpath

Brillouin zone: HEX





New Job Nov 14, 2022, 18:49 PM

project Default

Select Job Actions

SAVE

1. MATERIALS

2. WORKFLOW

3. COMPUTE



Compute

Runtime configuration parameters



Time limit

01:00:00

Time limit type

per single attempt

Cluster

master-vagrant-cluster-001.exabyte.io

See clusters status

Queue

debug (D)

Compute documentation

Nodes

1

Cores

1



Notifications

Click user icon to enable

demo
demo@mat3ra.com

Events

Choose events to trigger notifications

Started

Aborted

Ended





Default

accounting name demo-default
description: Default project



OVERVIEW

JOBS

Click to filter items below ...

 1-1 of 1 job 0 selected

NAME & WORKFLOW	APPLICATION	CLUSTER - QUEUE & CORES	RUN & WAIT TIME	STATUS	CREATED	SHARED	PUBLIC	EXT+LNK	EXT+WEB
New Job Nov 14, 2022, 18:49 PM Valence Bank Offset (2D)	espresso, python 5.4.0, 3.8.6	cluster-001 - D 1 node x 1 core	18m 10s 2s		Nov 14, 2022 6:52 pm				

 1-1 of 1 job 0 selected

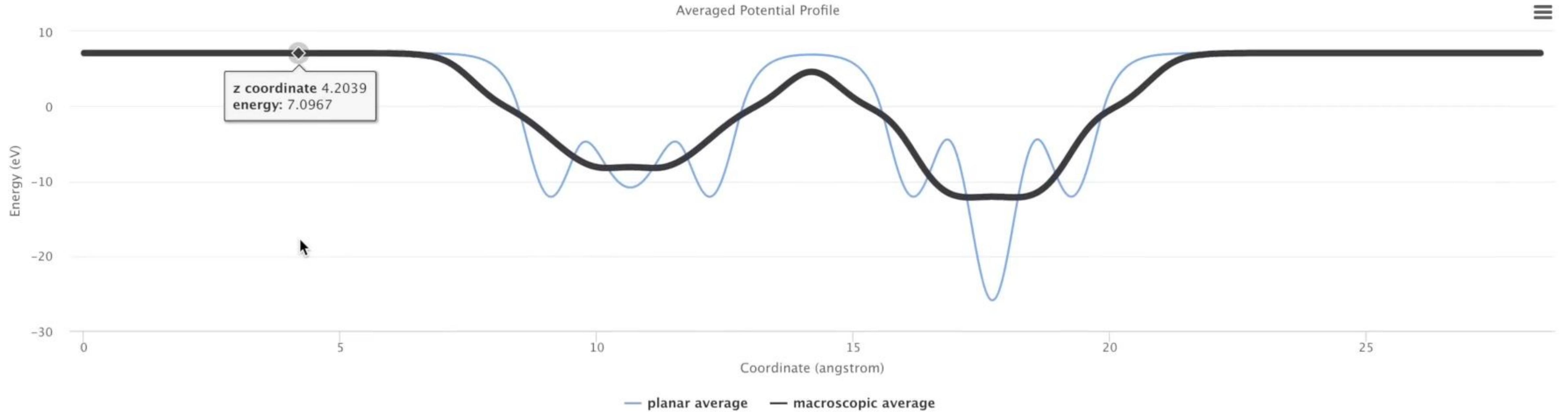


BS + Avg ESP (Interface) - average ESP

espresso

-

Averaged Potential Profile



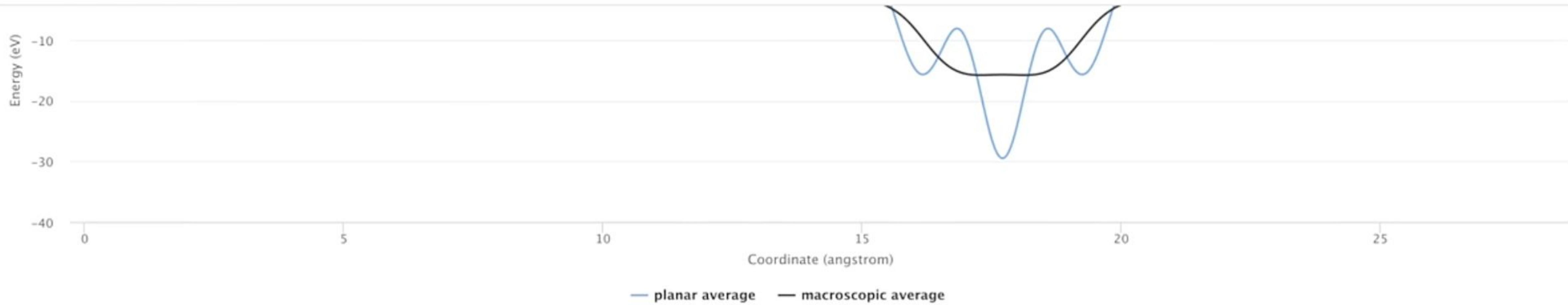
i



BS + Avg ESP (interface left) - pw_scf

espresso

-



Calculate VBO - Valence Band Offset

python



-



Valence band offset (eV)



0.268



platform.mat3ra.com/exadmin/projects#properties

Home > Account

Mat3ra

description: Joined on Jul 17, 2024

BIO PROJECTS MATERIALS PROPERTIES WORKFLOWS JOBS SERVICE LEVELS PREFERENCES

band

Advanced

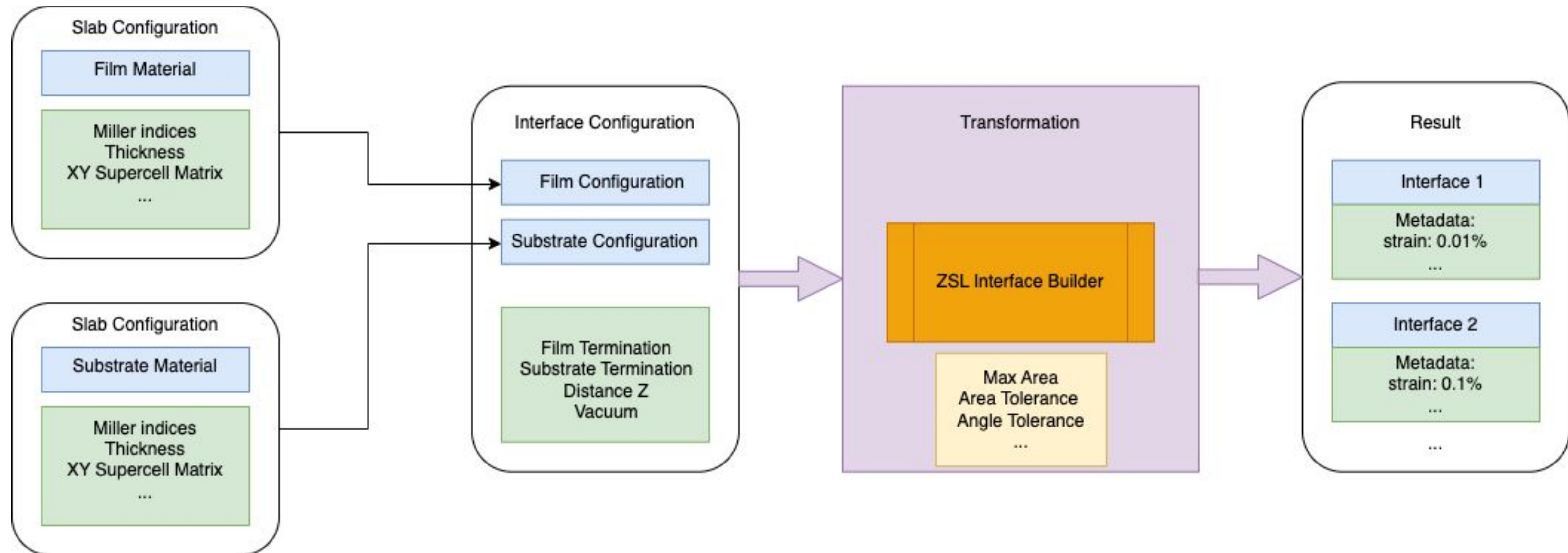
Icon	Name	Unit	Value	Material	Material Formula	Job	Engine	Version	Model	Groups	Method	Subtype	Precision	Actions
	Band structure				SrZrO3		vasp	5.4.4	dft	gga:pbe	pseudopotential	paw	2000	
	Band gaps (direct/indirect)	eV	2.299 / 0.802	-			shell	4.2.46	unknown	unknown	unknown	unknown		
	Band structure			-			shell	4.2.46	unknown	unknown	unknown	unknown		
	Band structure				SrZrO3		vasp	5.4.4	dft	gga:pbe	pseudopotential	paw	2000	
	Band structure				SrZrO3		vasp	5.4.4	dft	gga:pbe	pseudopotential	paw	2000	
	Band structure				SrZrO3		vasp	5.4.4	dft	gga:pbe	pseudopotential	paw	2000	
	Band structure				SrZrO3		vasp	5.4.4	dft	gga:pbe	pseudopotential	paw	2000	
	Band structure				SrZrO3		vasp	5.4.4	dft	gga:pbe	pseudopotential	paw	2000	
	Band gaps (direct/indirect)	eV	3.140 / 1.050	-			espresso	6.3	dft	gga:pbe	pseudopotential	us	1024	
	Band structure			-			espresso	6.3	dft	gga:pbe	pseudopotential	us	1024	
	Band gaps (direct/indirect)	eV	3.140 / 2.060	-			espresso	6.3	dft	qqa:pbe	pseudopotential	us	1024	

Rows per page: 20 < 1–20 of 37 >

**UPCOMING: Mat3ra 2D -
product line focused on layers,
heterostructures, interfaces**

Design of interfaces and layered compounds

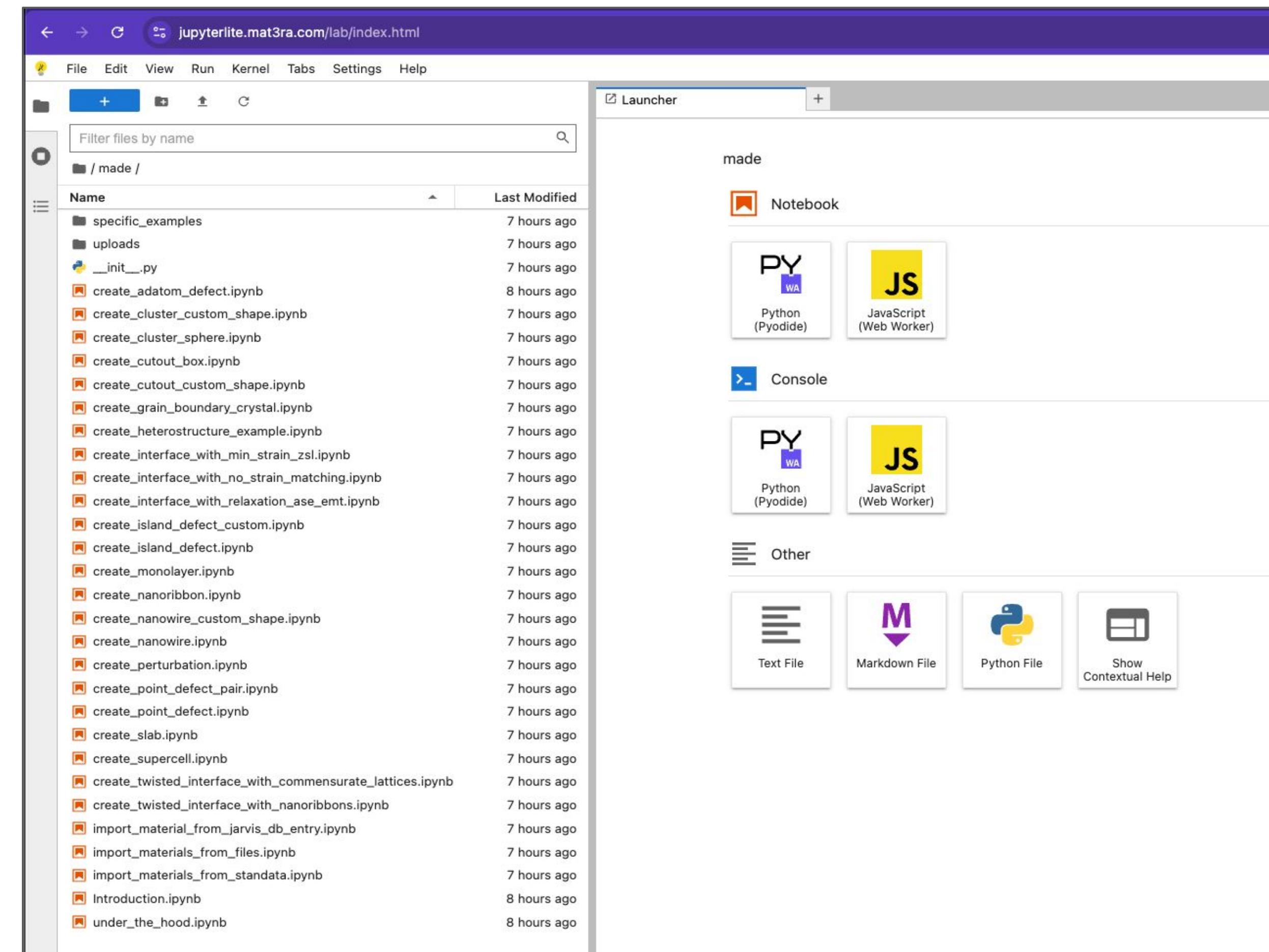
Process Diagram: creating an Interface



Supported Material Categories

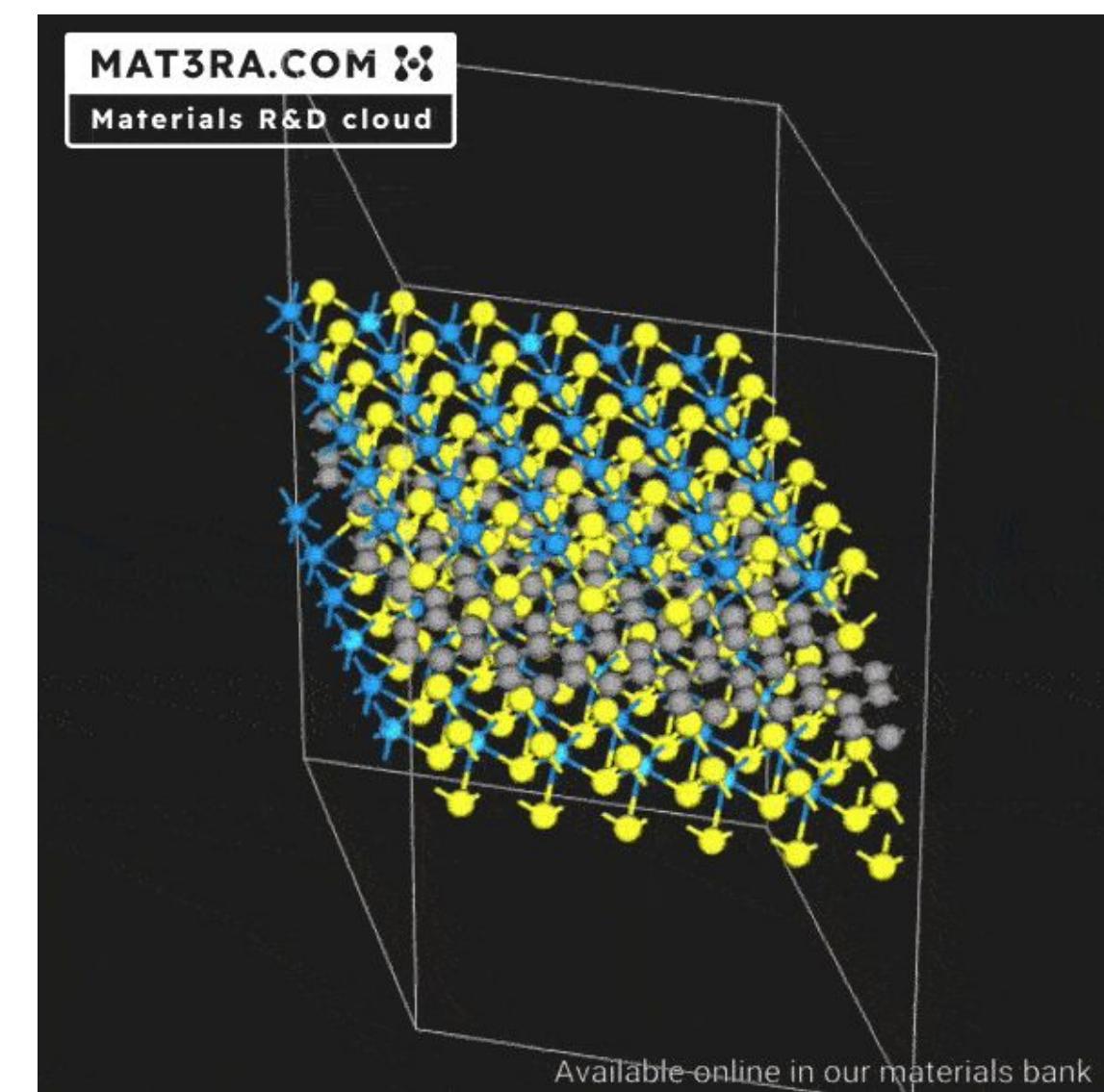
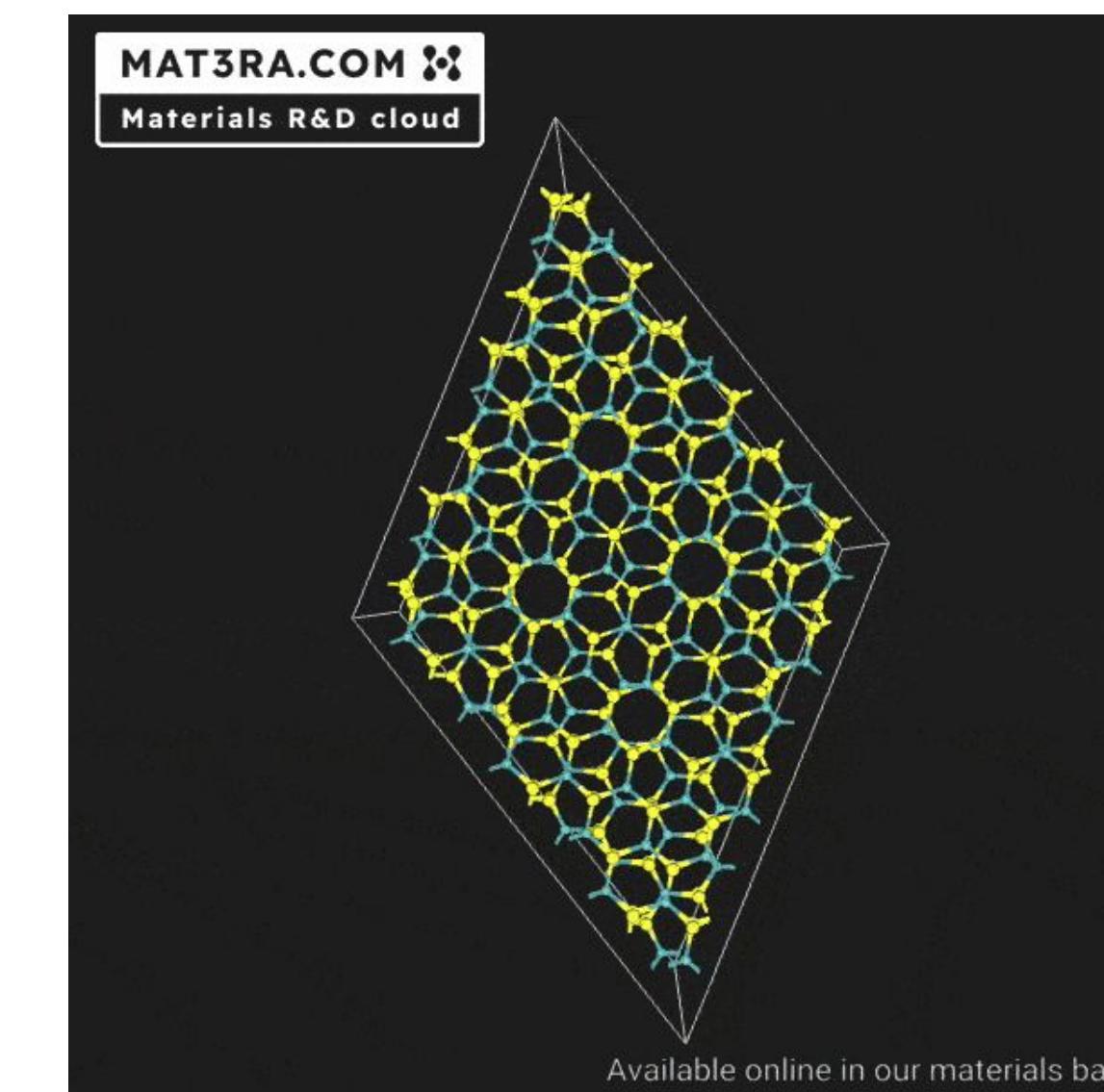
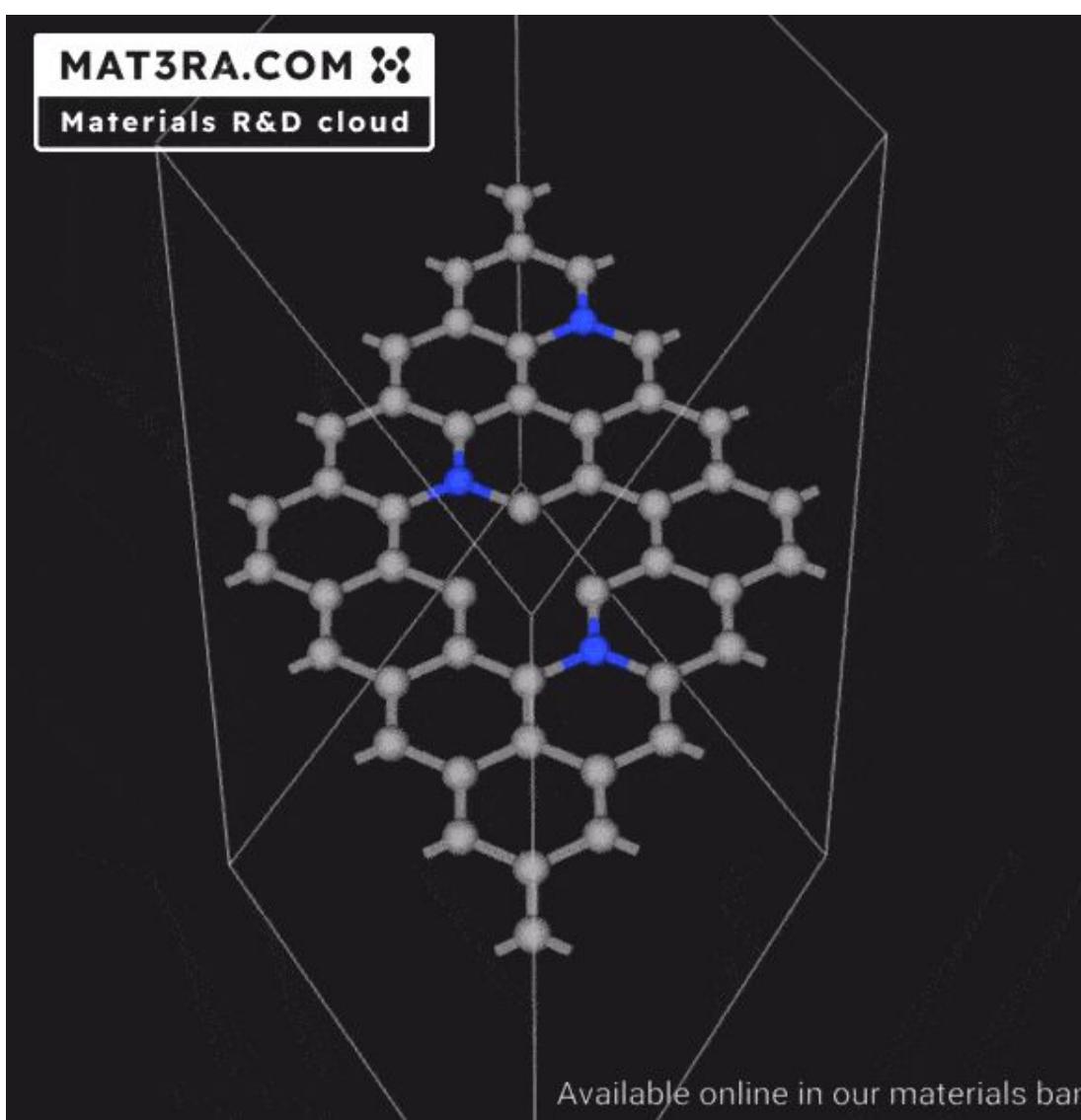
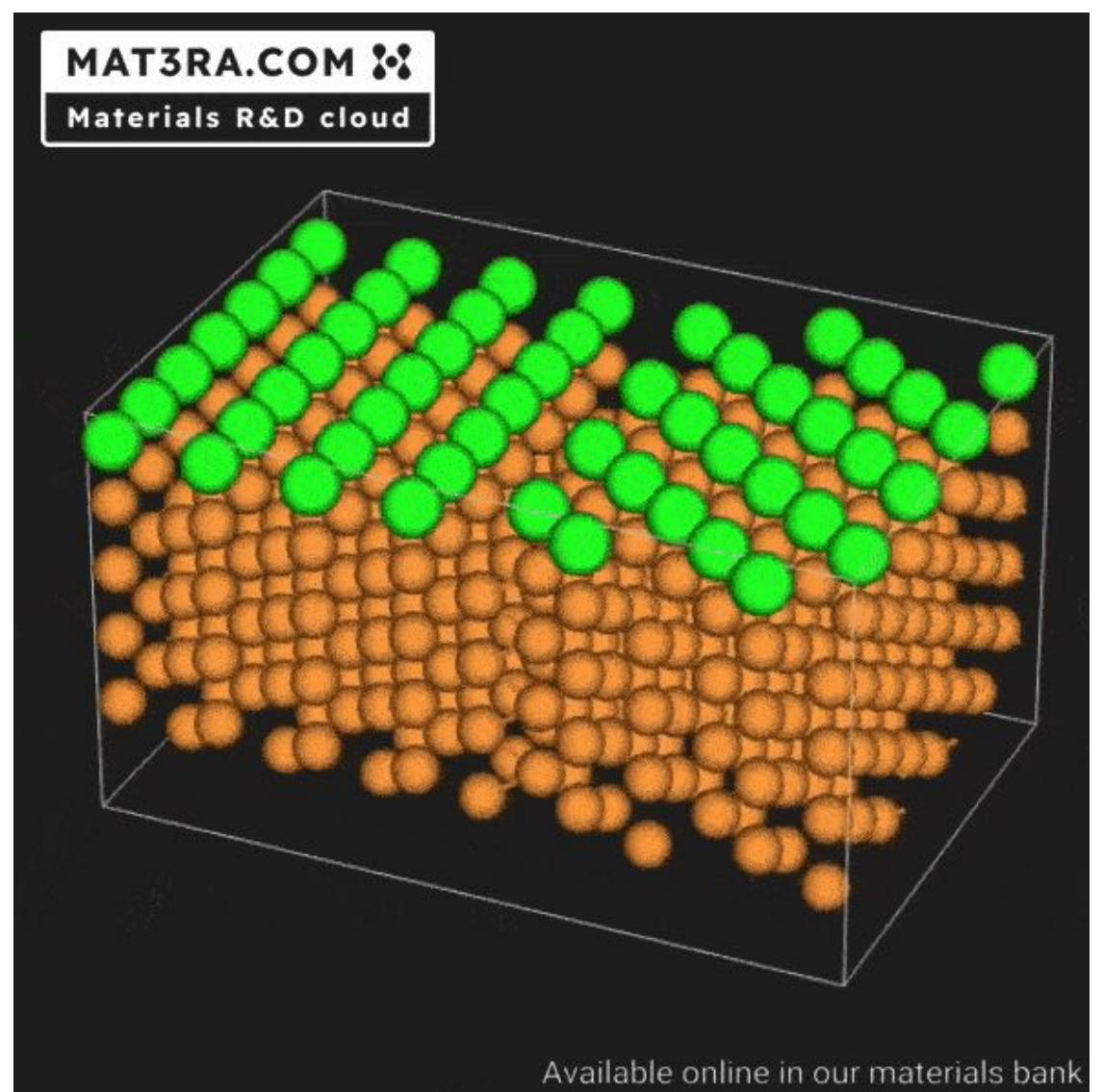
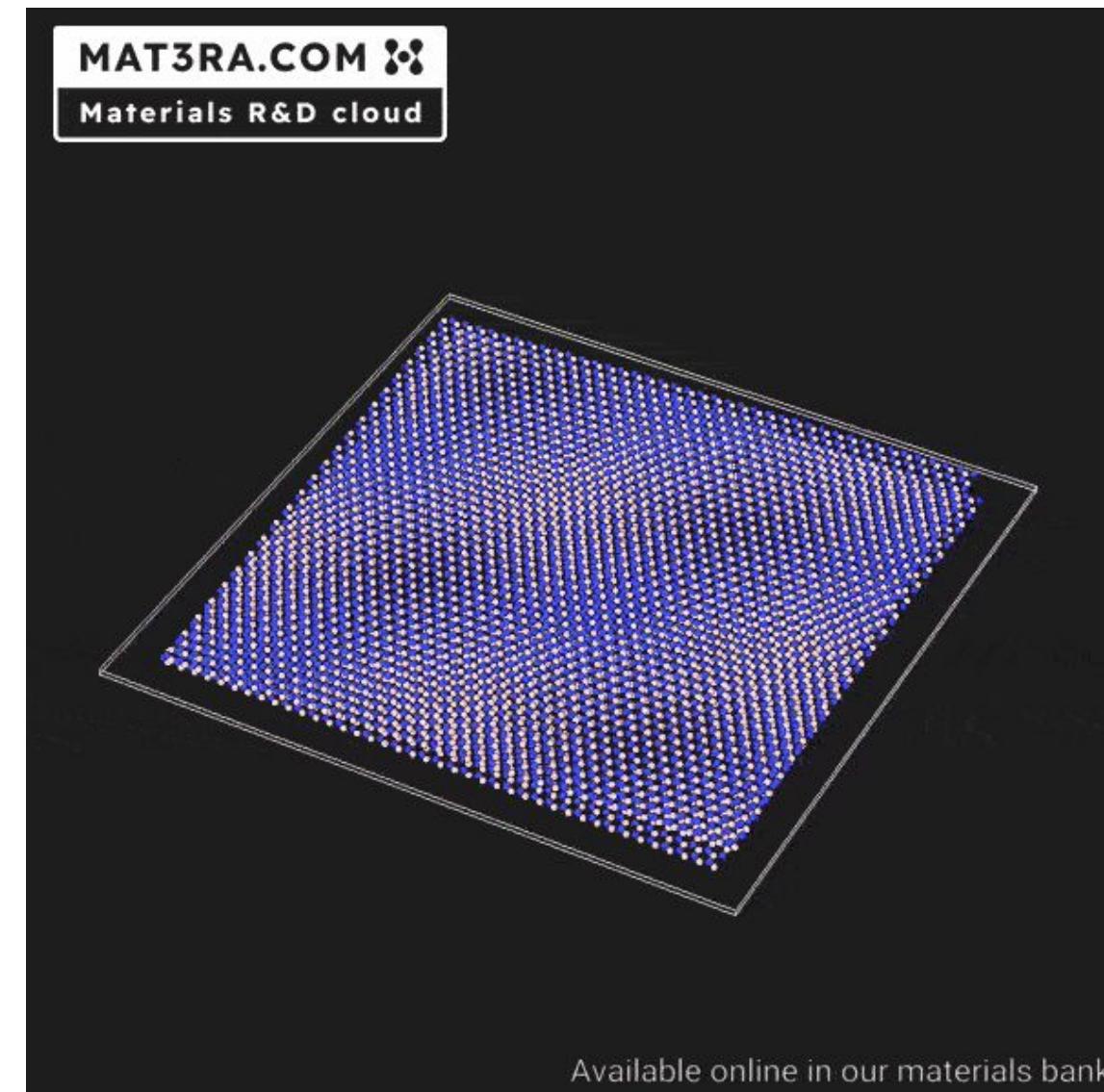
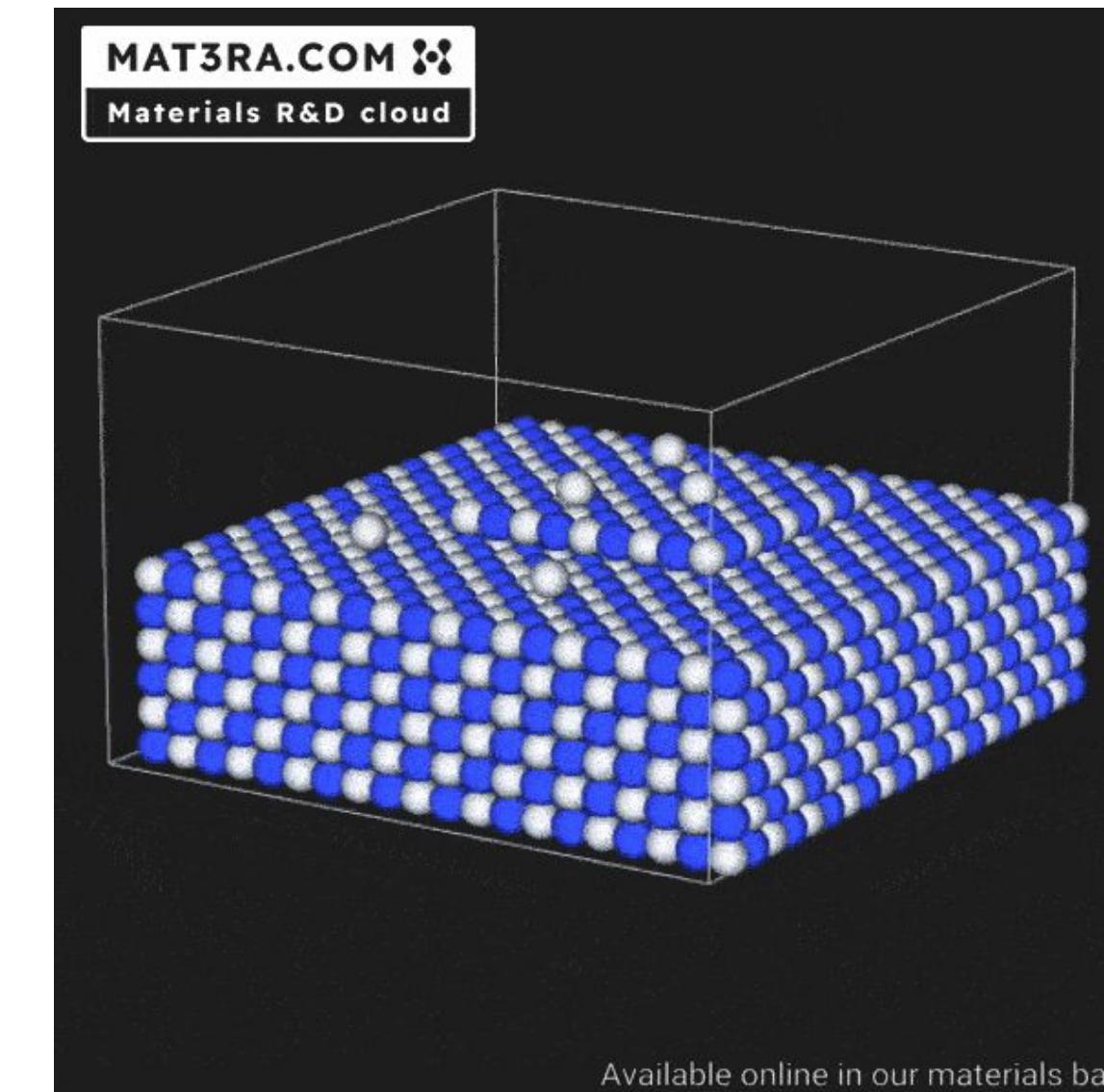
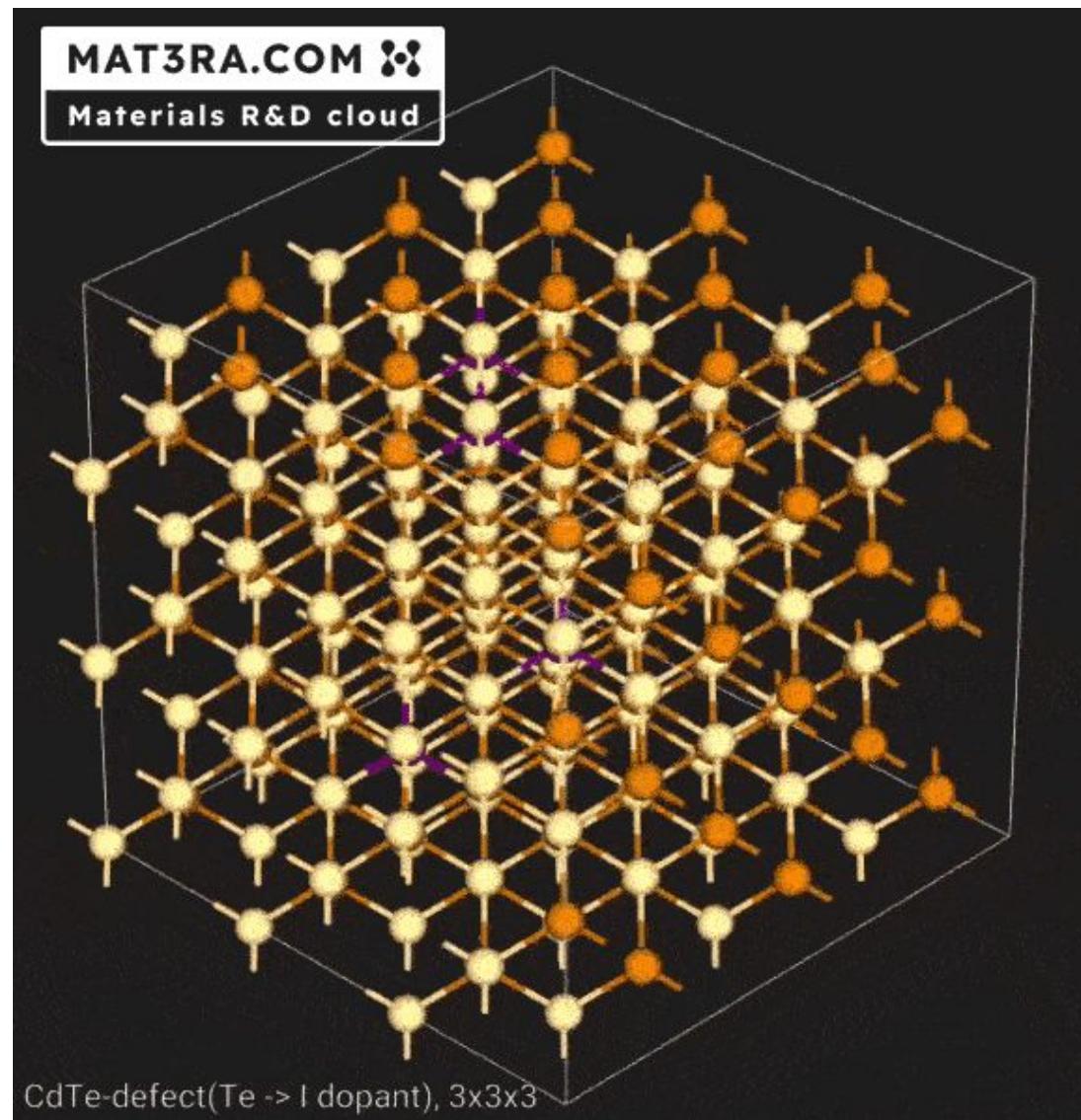
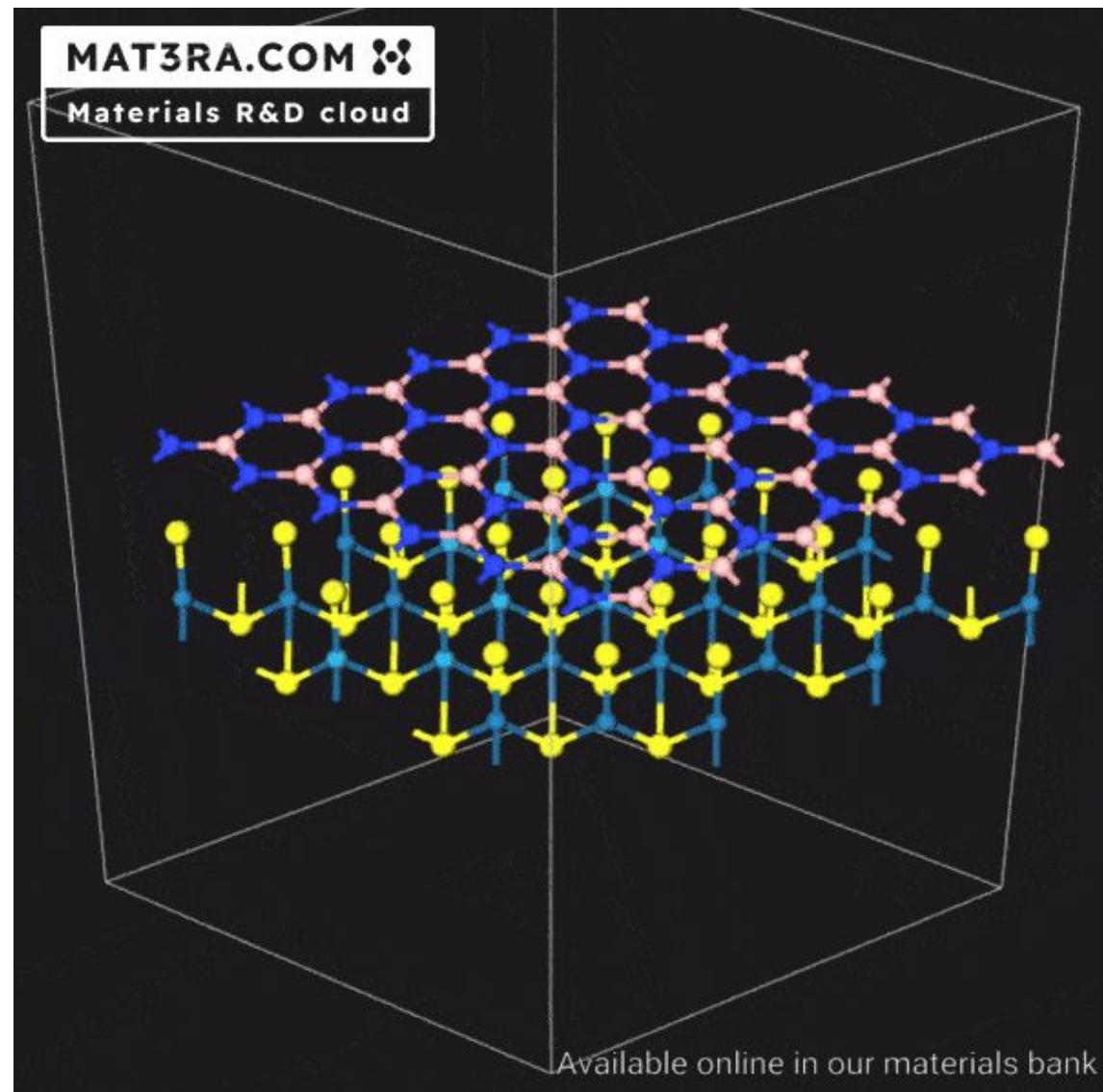
Domain	Subdomain	Subsubdomain
Single Material Structures	3D Structures	Crystal Supercell
	2D Structures	Slab Monolayer
	1D Structures	Nanotube Nanowire
	0D Structures	Nanoribbon Cluster / Sphere Box-cutout Custom-shape
Multi-Material Structures	Interfaces	2D+2D, 2D+3D, 3D+3D
	Stacked Nanoribbons	Twisted Nanoribbons
	Heterostructures	Heterostructure with consecutive interfaces
Defects	Point Defects (0D)	Vacancy Substitution Interstitial Defect Pair
	Surface Defects (2D)	Adatom Island Terrace
	Planar Defects (3D)	Grain Boundary in Crystal (3D) Grain Boundary in Slab (2D) Grain Boundary on 2D
Passivation	Surface Passivation	Slab Passivation
	Edge Passivation	Nanoribbon Passivation
Perturbations		Simple Distance-preserving

Notebooks for typical uses: jupyterlite.mat3ra.com

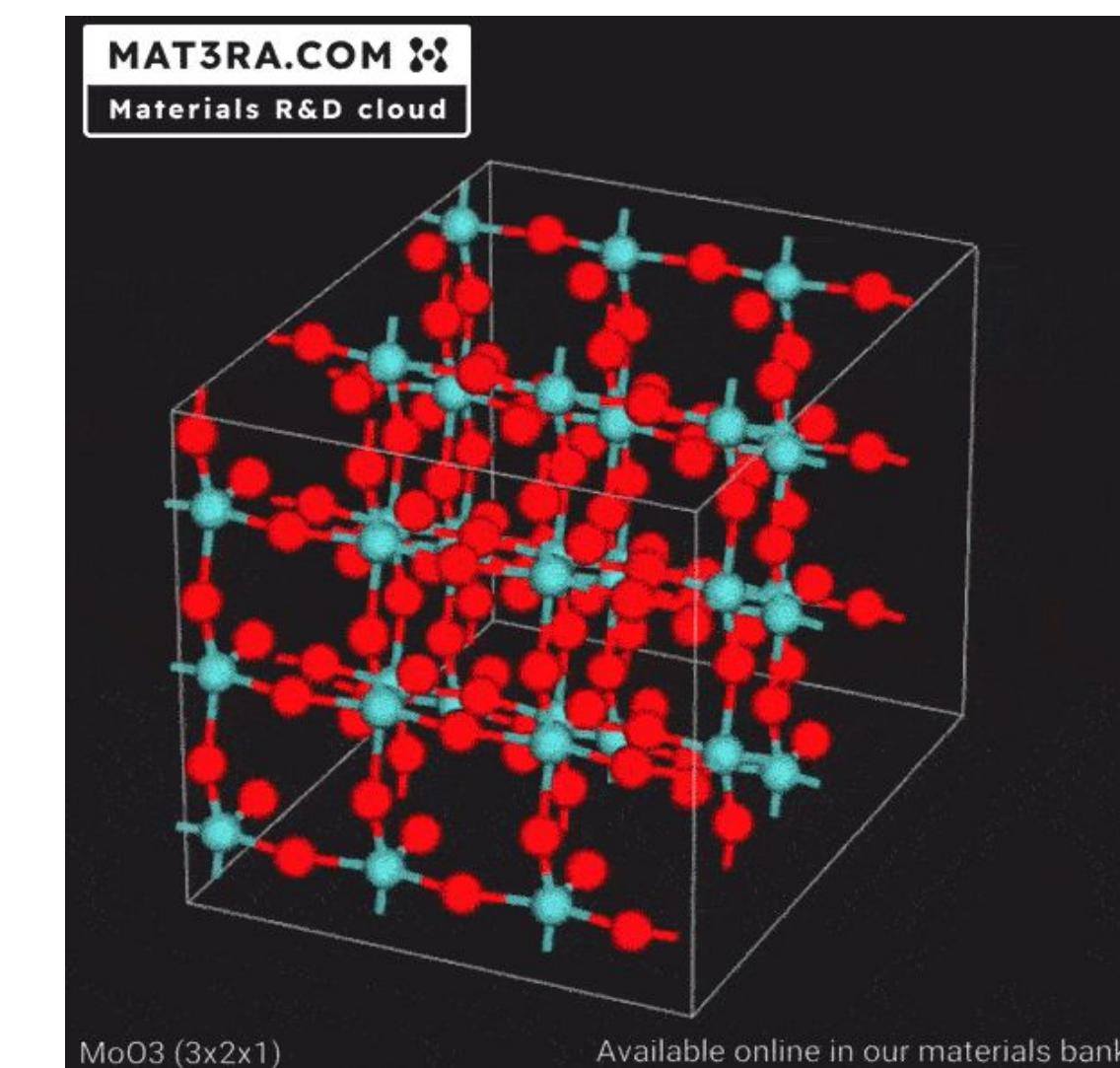
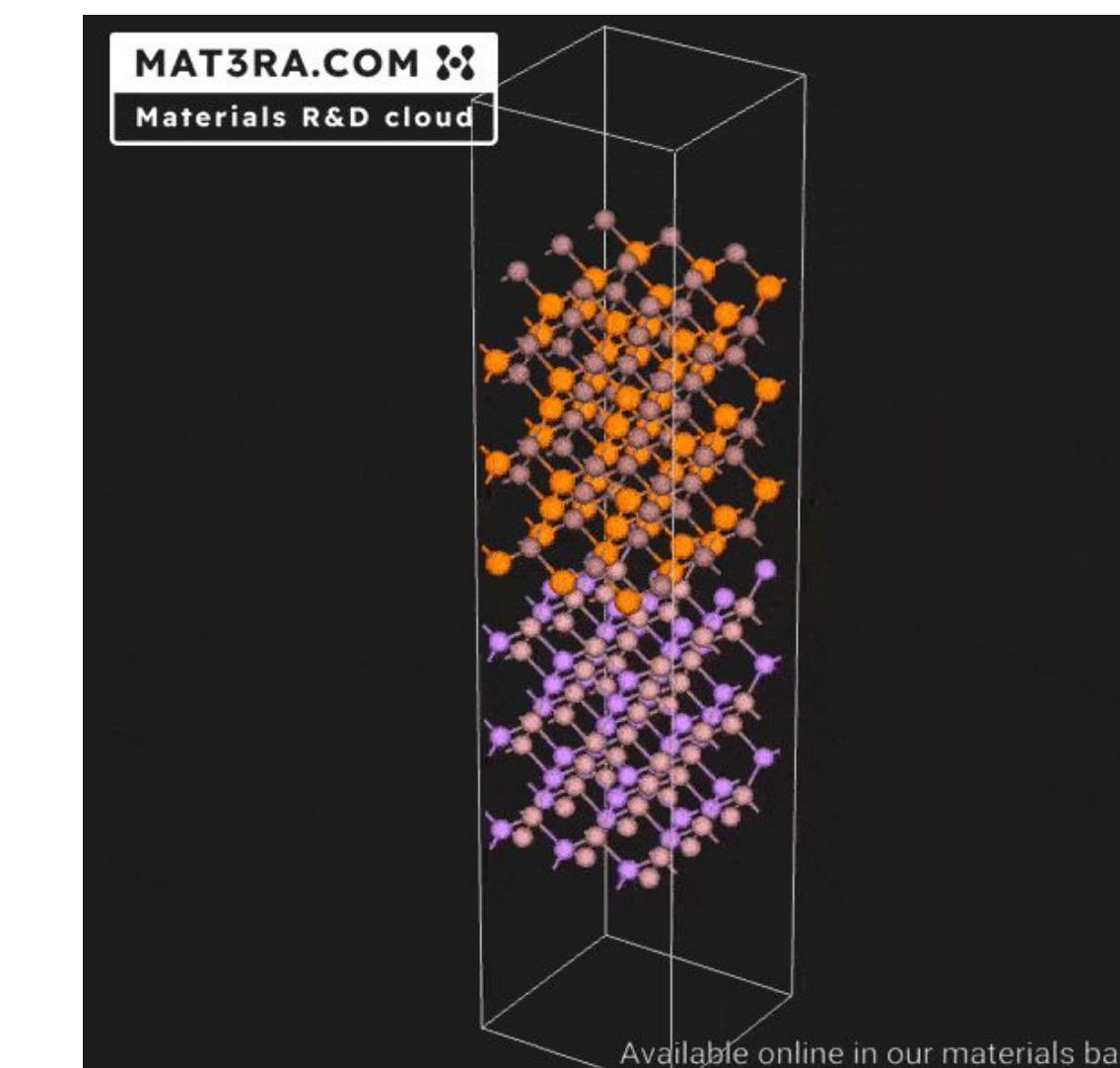
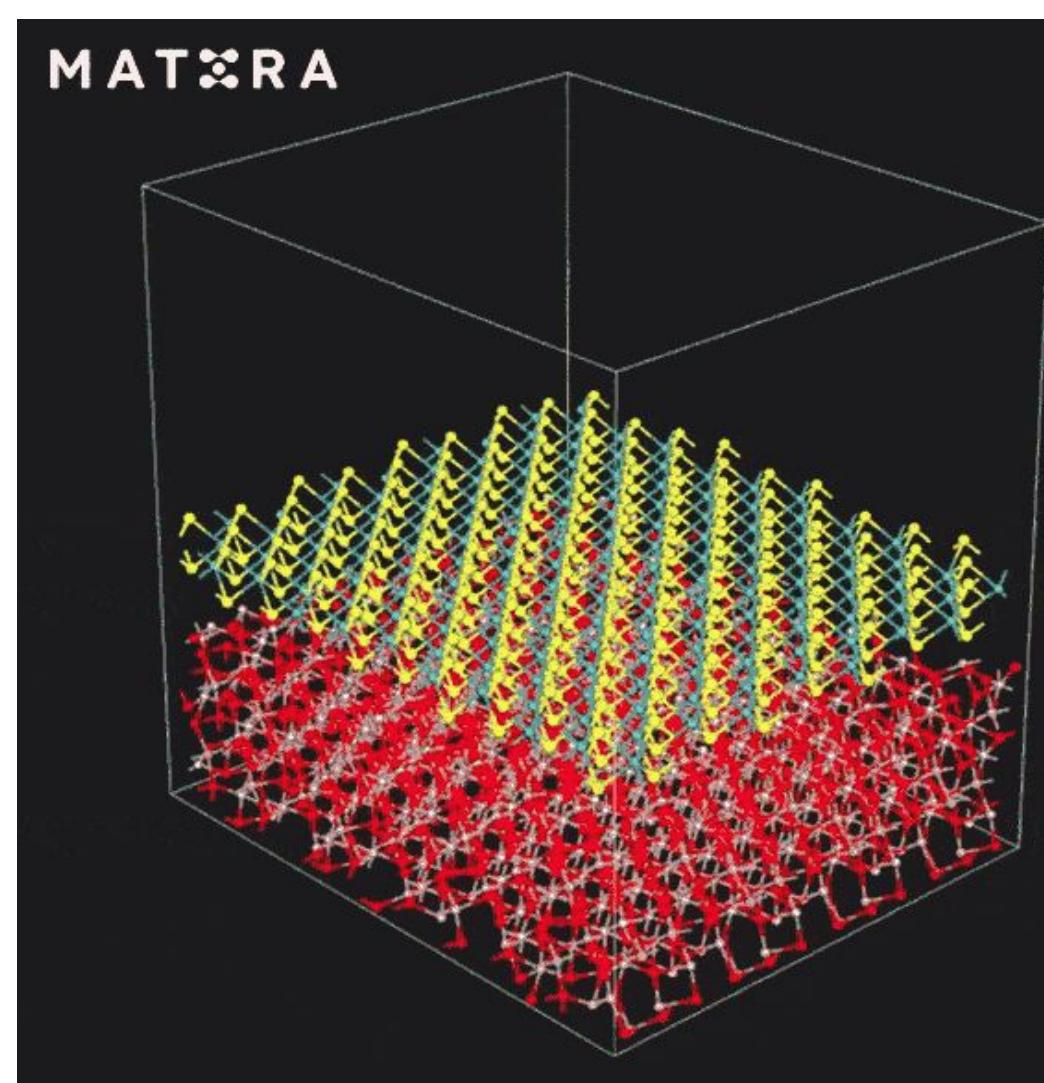
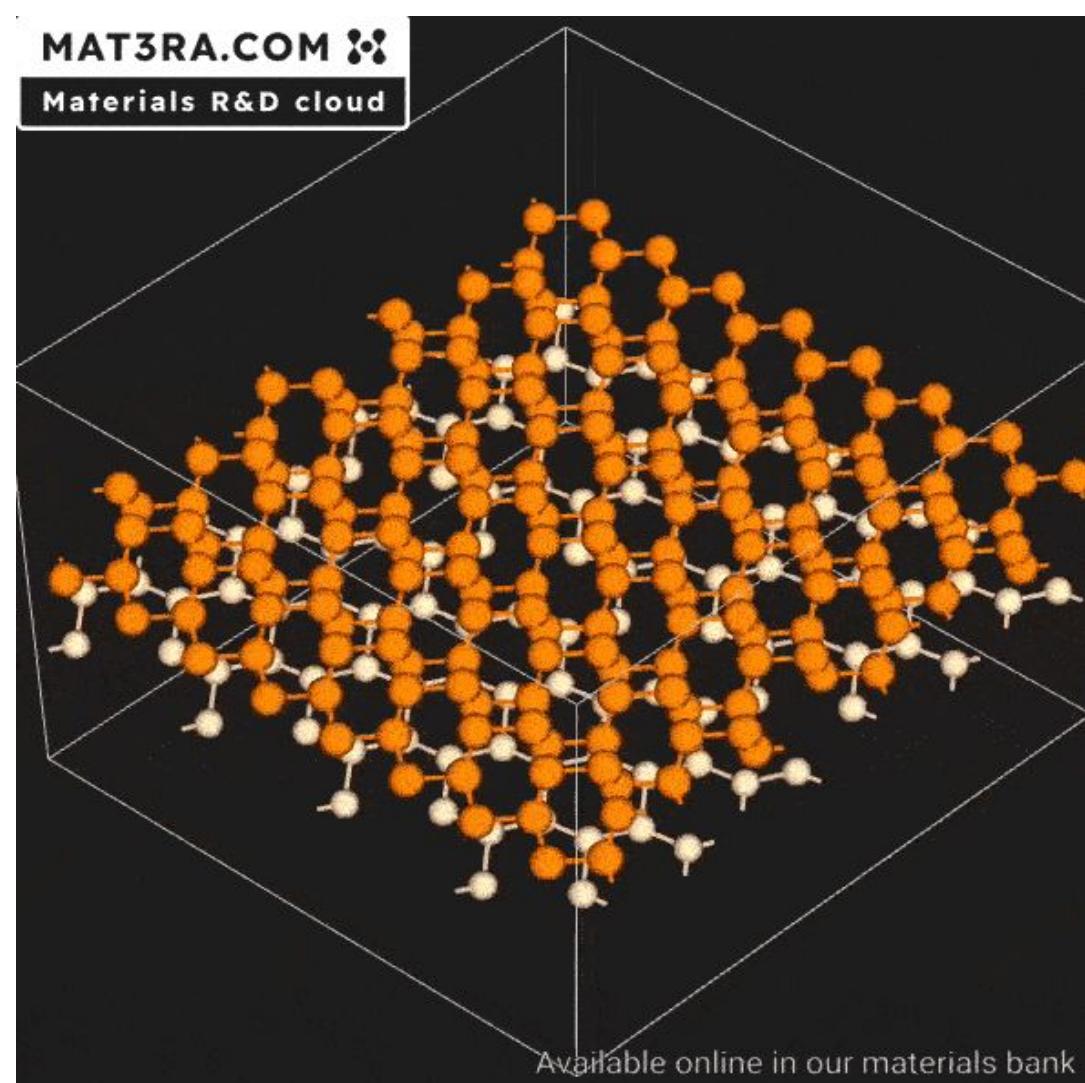
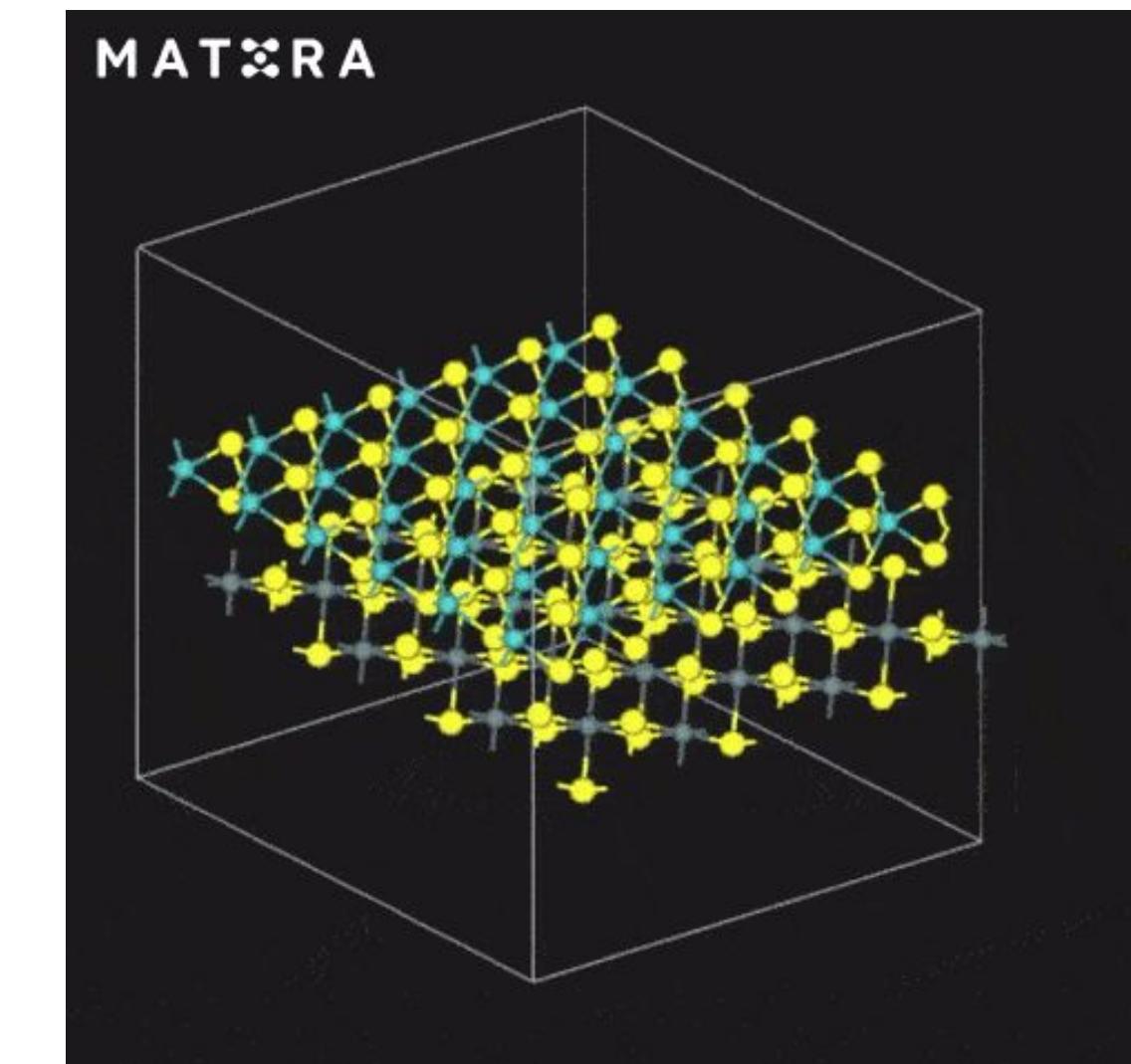
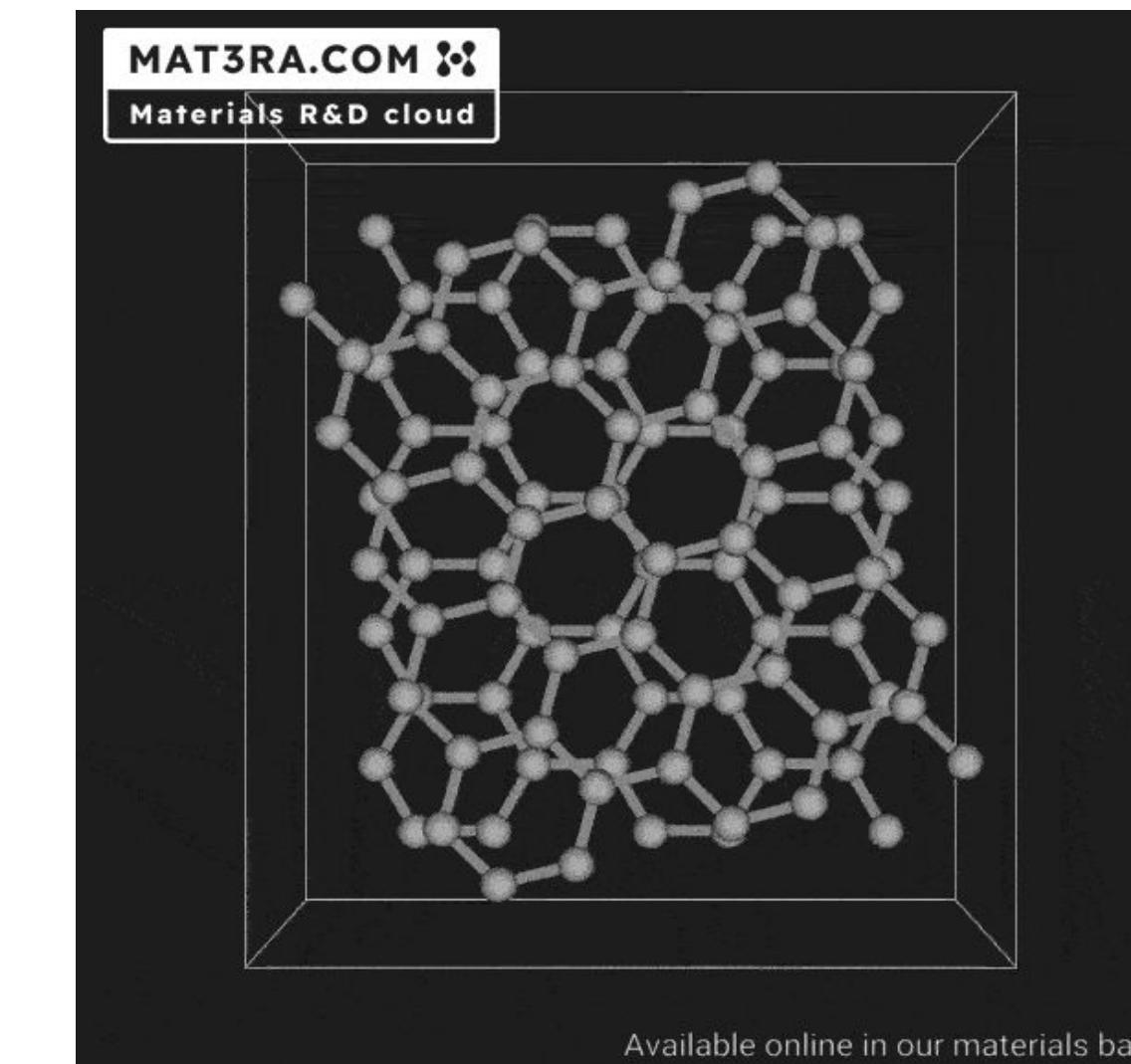
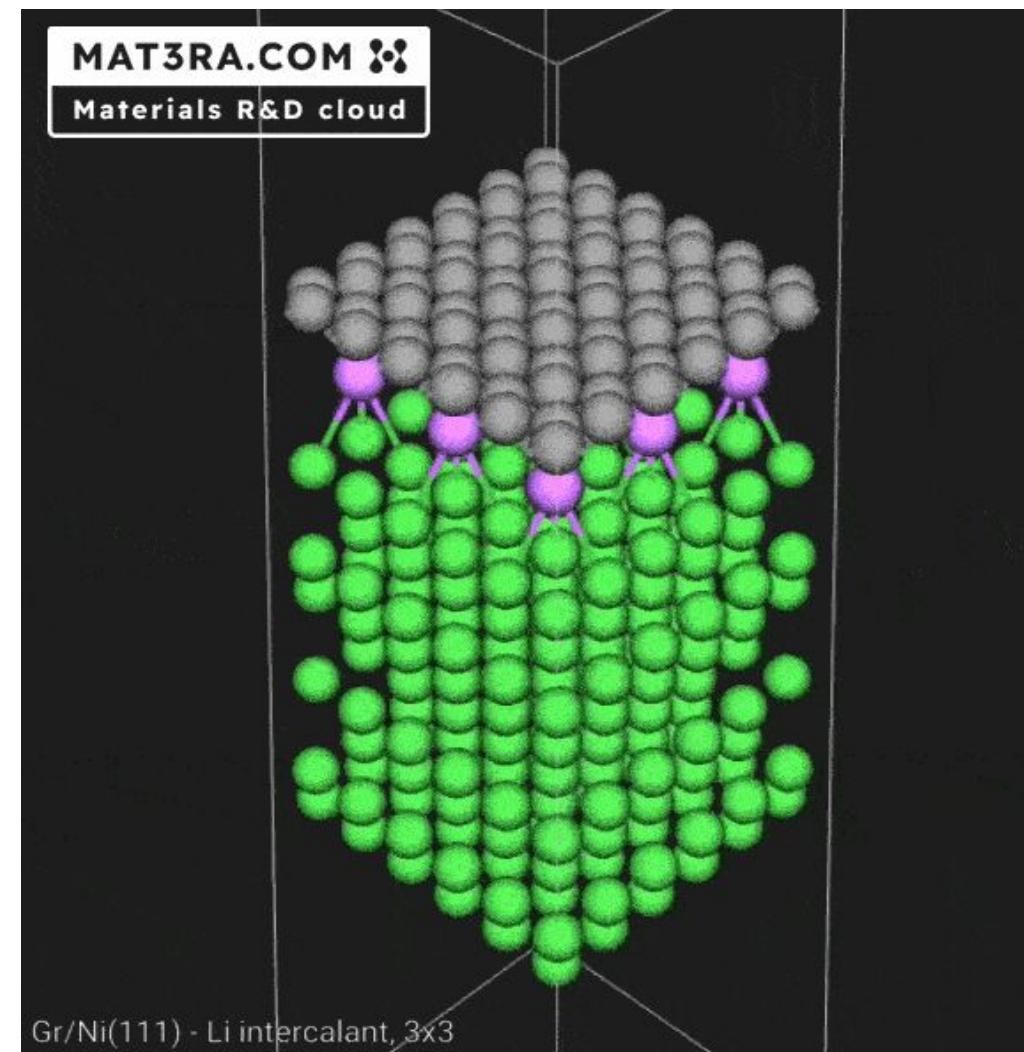
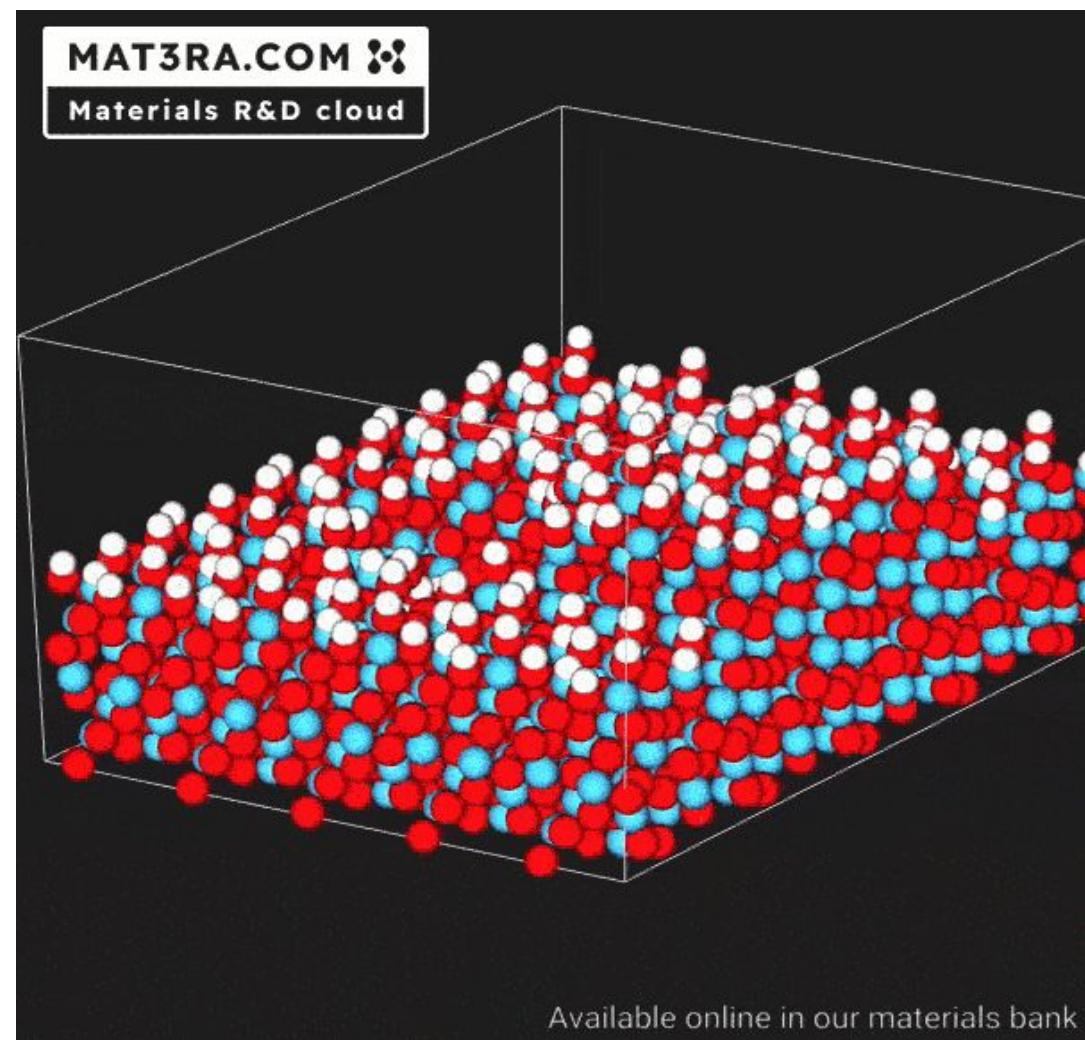


Materials Designer Web-App: <https://mat3ra-materials-designer.netlify.app/>

Resulting Materials Structures



Resulting Materials Structures



Extra: REST-API USAGE EXAMPLE

Files

dev

Go to file t

- > .github
- > examples
- > extra
- > images
- > other
 - > assets
 - > experiments
 - > jarvis
 - import_material_from_jarvis...
 - run_job_using_material_fro...
 - > job
 - > machine_learning
 - > materials_designer
 - > materialsproject
 - > python_transformations
 - > webinar
 - __init__.py
 - > packages
 - > scripts
 - > utils
 - .gitattributes
 - .gitignore
 - .lycheeignore
 - .pre-commit-config.yaml
 - README.ipynb
 - README.md
 - config.yml

api-examples / other / jarvis / run_job_using_material_from_jarvis_db.ipynb

Preview Code Blame 574 lines (574 loc) · 15.3 KB

Raw ⌂ ⌄ ⌅ ⌆ ⌇ ⌈ ⌉ ⌋ ⌊ ⌊

Create a simple heterostructure

We use two material ids and place them one above another.

```
In [ ]:
from jarvis.core.atoms import Atoms
from jarvis.analysis.interface.zur import make_interface

## Note: JVASP-670 is an entry for MoTe2
jid1 = "JVASP-670"
jid2 ="JVASP-664"

for i in dft_2d:
    if i["jid"] == jid1:
        atoms1 = Atoms.from_dict(i["atoms"])
for i in dft_2d:
    if i["jid"] == jid2:
        atoms2 = Atoms.from_dict(i["atoms"])

interface_atoms_dict = make_interface(film=atoms1, subs=atoms2)
heterostructure_atoms = interface_atoms_dict["interface"].center_around_origin()

print (jid1,jid2,atoms1.composition.reduced_formula,atoms2.composition.reduced_formula, heterostructure_atoms)
```

Extract the film and substrate

```
In [ ]:
# Using the fractional coordinate Z level of 0.5 to separate top/bottom
# See also https://github.com/usnistgov/jarvis/issues/311
heterostructure_atoms_copy = Atoms.from_dict(heterostructure_atoms.to_dict())
indices_to_remove = []
for index, coord in enumerate(heterostructure_atoms_copy.coords):
    print(coord, index)
    if coord[2] < 0.5:
        indices_to_remove.append(index)
for i, ind in enumerate(indices_to_remove):
    heterostructure_atoms_copy = heterostructure_atoms_copy.remove_site_by_index(ind - i)
    print("removed", ind, heterostructure_atoms_copy.props)
substrate_atoms = Atoms.from_dict(heterostructure_atoms_copy.to_dict())

heterostructure_atoms_copy = Atoms.from_dict(heterostructure_atoms.to_dict())
indices_to_remove = []
for index, coord in enumerate(heterostructure_atoms_copy.coords):
    print(coord, index)
    if coord[2] > 0.5:
        indices_to_remove.append(index)
for i, ind in enumerate(indices_to_remove):
    heterostructure_atoms_copy = heterostructure_atoms_copy.remove_site_by_index(ind - i)
    print("removed", ind, heterostructure_atoms_copy.props)
film_atoms = Atoms.from_dict(heterostructure_atoms_copy.to_dict())
```

The screenshot shows a Jupyter Notebook interface with a file browser on the left and a Colab notebook on the right.

File Browser:

- Left sidebar: A file browser showing a folder structure under "/api/job/".
- Content area: A table listing files with columns "Name" and "Last Modified".
- Selected file: "run-simulations-and-extract-properties.ipynb" (3 months ago).

Colab Notebook:

- Title bar: "Launcher" and "run-simulations-and-extract-properties.ipynb" (Python (Pyodide)).
- Header: "File", "Edit", "View", "Run", "Kernel", "Tabs", "Settings", "Help".
- Toolbar: Standard Colab toolbar icons.
- Content area:
 - Google colab logo.
 - ## Run Simulations and Extract Properties
 - This example demonstrates how to use Mat3ra RESTful API to create simulation [Jobs](#) programmatically for multiple [Materials](#) at once and extract the resulting [Properties](#) forming a [Pandas](#) dataframe.
 - This approach can work with any [Workflows](#). For the demonstration purpose we use the Density Functional Theory and extract Electronic Band Gap as the property of interest.
 - IMPORTANT NOTE:** In order to run this example in full, an active Mat3ra.com account with access to VASP (Vienna ab-initio simulations package) is required. Alternatively, Readers may substitute the workflow ID below with another one (an equivalent one for Quantum ESPRESSO, for example) and adjust extraction of the results ("Extract results" section). RESTful API credentials shall be updated in [settings](#).

Steps

We follow the below steps:

- Import materials from [Materials Bank](#)
- Group imported materials inside a [materials set](#)
- Create jobs for the materials and grouping them inside a [jobs set](#)
- Submit jobs and monitoring the progress
- Extract the [final structure](#) (relaxed structure) and its properties
- Output the results as Pandas DataFrame

OPEN IN BROWSER

Use cases 4 STEM (Sergei Kalinin, Utkarsh Pratiush)

Connecting Experiment and Theory

Is about connecting people first



Connecting Experiment and Theory

Extract and store atomic structures

The screenshot shows a GitHub repository interface for the 'pyAutoMic' project under the 'pycroscopy' organization. The repository path is 'pyAutoMic / TEM / stemOrchestrator / notebooks / mat3ra / ondrej_graphene_to_poscar.ipynb'. A commit by 'utkarshp1161' titled 'add: onderj-graphene-to-poscar-mat3ra' was made 2 weeks ago with commit hash 'dd19d5e'. The notebook has 409 lines (409 loc) and is 11.7 KB in size. The 'Preview' tab is selected. The main content of the notebook is displayed below:

Creating POSCAR Files from DCNN-Detected STEM Coordinates and sending to mat3ra servers

This notebook demonstrates how to convert DCNN-predicted atomic coordinates into a POSCAR format, which can be used for DFT simulations using ASE or VASP.

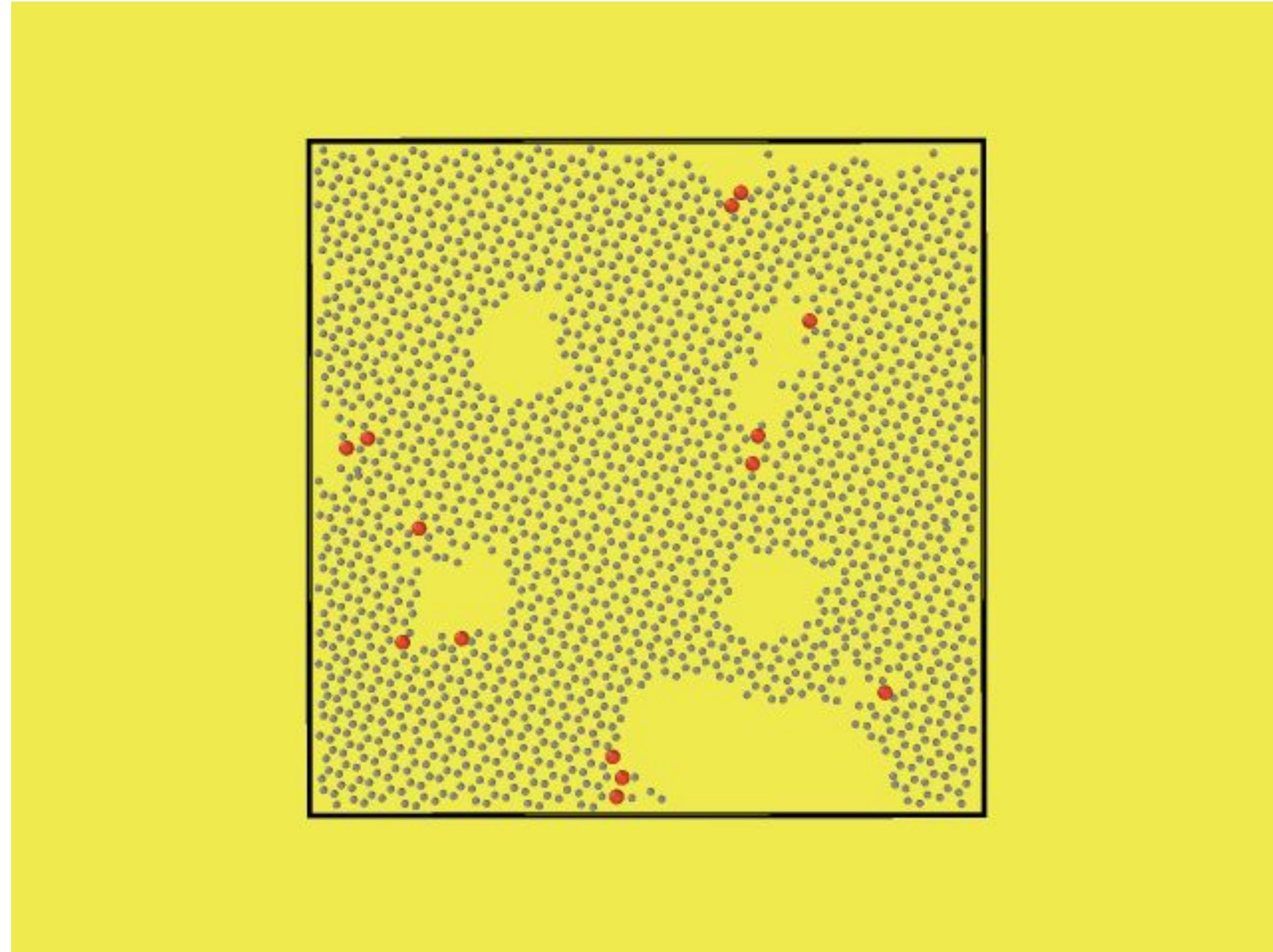
data credits: - [Ondej Dyck - ORNL](#)

Assumptions

- The atomic positions from `lattice_coord` are 2D (x, y).
- All atoms lie on a fixed plane ($z = 0 \text{ \AA}$ by default).
- The system is periodic or semi-periodic in the X-Y plane.
- Cell size can be derived from image dimensions or manually set.
- Output will be compatible with ASE and VASP.

Connecting Experiment and Theory

Extract and store atomic structures



Connecting Experiment and Theory

Extract and store atomic structures

The screenshot shows a Jupyter Notebook interface with the following details:

- Title Bar:** Shows the URL `github.com/pycroscopy/pyAutoMic/blob/main/TEM/stemOrchestrator/notebooks/mat3ra/ondrej_graphene_to_poscar.ipynb`.
- Header:** Includes a back button, forward button, refresh button, and a main dropdown menu.
- Breadcrumbs:** Displays the notebook's path: `pyAutoMic / TEM / stemOrchestrator / notebooks / mat3ra / ondrej_graphene_to_poscar.ipynb`.
- Toolbar:** Contains buttons for Preview, Code, Blame, 409 lines (409 loc) · 11.7 KB, Raw, and other file operations.
- Section Header:** "Sending to Mat3RA servers"
- Code Cells:** Five cells are visible:
 - Cell 1: Imports `yaml` and reads a YAML file named `credential.yaml`. It extracts `ACCOUNT_ID`, `AUTH_TOKEN`, and `OWNER_ID`.
 - Cell 2: Imports `sys` and `os`, and appends a path to a local directory.
 - Cell 3: Imports `ENDPOINT_ARGS` from `utils.settings` and `display_JSON` from `utils.generic`. It also imports `MaterialEndpoints` from `exabyte_api_client.endpoints.materials`.
 - Cell 4: Sets `ENDPOINT_ARGS` to the value of `cred["endpointArgs"]`.
 - Cell 5: Creates an instance of `MaterialEndpoints` using the arguments from Cell 4.

Connecting Experiment and Theory

Extract and store atomic structures

Home > Utkarsh Pratiush

Utkarsh Pratiush
utkarsh
description:Joined on Jan 29, 2023

BIO PROJECTS MATERIALS PROPERTIES WORKFLOWS JOBS

Advanced

	Name	Formula	Unit Cell Formula	Lattice	Symmetry	Tags	Created	Actions
<input type="checkbox"/>	C_Si_32	Si16C1573	Si16 C1573	TET	Pm		05-05-2025 11:17	⋮
<input type="checkbox"/>	C_Si_32 (modified by admin)	Si16C1573	Si16 C1573	TET	Pm		05-05-2025 11:17	⋮
<input type="checkbox"/>	C_Si_20	Si13C903	Si26 C1806	TET	Pm		05-05-2025 11:17	⋮
<input type="checkbox"/>	C_Si_43	Si19C1426	Si19 C1426	TET	Pm		05-05-2025 11:17	⋮
<input type="checkbox"/>	C_Si_16	Si11C914	Si22 C1828	TET	Pm		05-05-2025 11:16	⋮
<input type="checkbox"/>	C_Si_08	Si11C976	Si22 C1952	TET	Pm		05-05-2025 11:16	⋮
<input type="checkbox"/>	C_Si_04	Si23C1975	Si23 C1975	TET	Pm		05-05-2025 11:16	⋮
<input type="checkbox"/>	C_Si_41	Si19C1428	Si19 C1428	TET	Pm		05-05-2025 11:16	⋮

Rows per page: 100 < 1-61 of 61 >

Connecting Experiment and Theory

Extract and store atomic structures

Home > Utkarsh Pratiush > Materials - C_Si_01 (Modified by admin)

C_Si_01 (Modified by admin)
formula Si₁₇C₂₀₀₂ lattice TET

Description Select Material Actions SAVE & EXIT

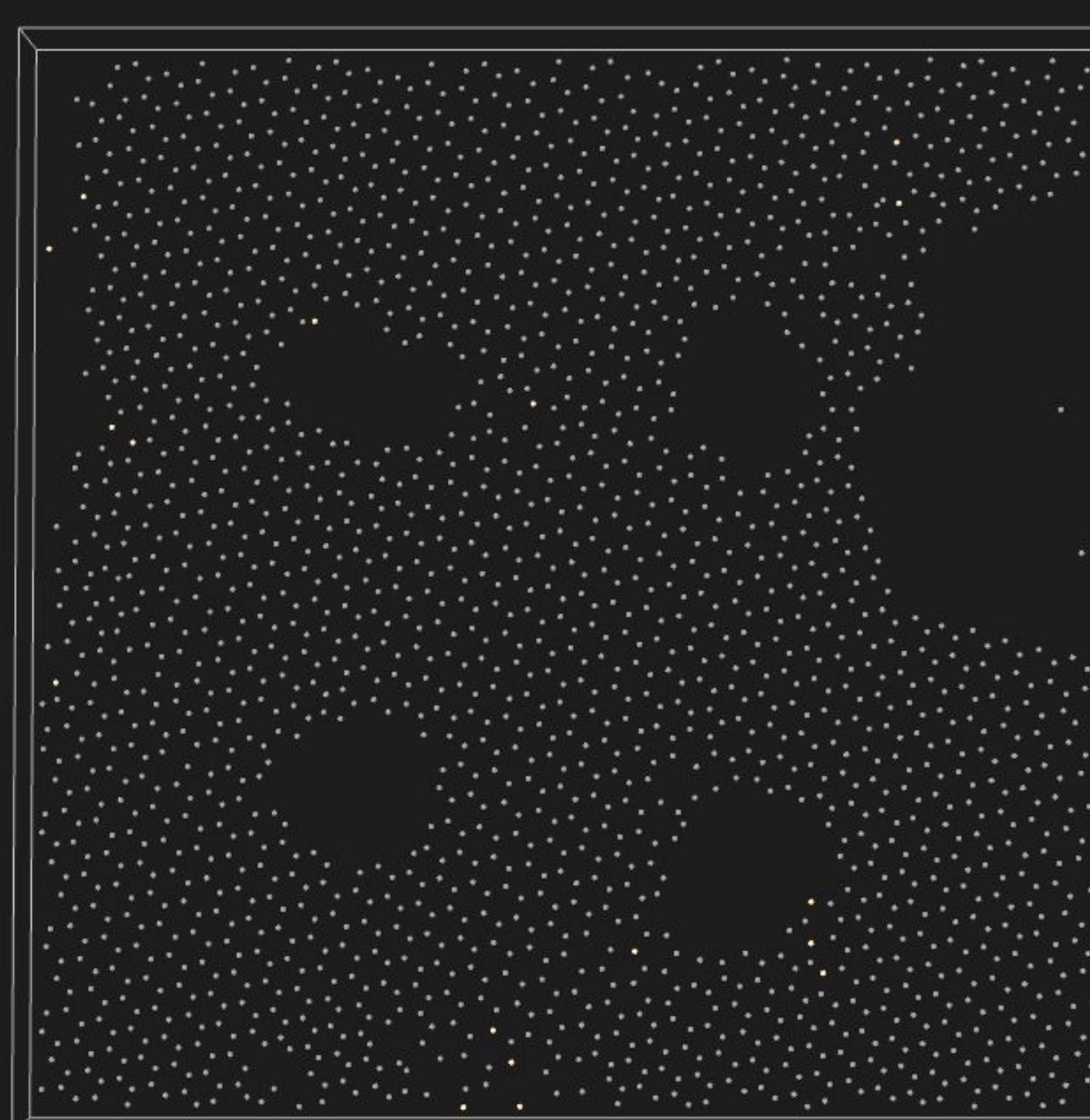
Lattice
TET

a	96.000	b	96.000	c	10.000
a	90.000	β	90.000	γ	90.000

Basis

1 C	0.107100	0.010100	0.000000
2 C	0.047900	0.011700	0.000000
3 C	0.210900	0.011700	0.000000
4 C	0.289100	0.012700	0.000000
5 C	0.980200	0.010600	0.000000
6 C	0.417000	0.013700	0.000000
7 C	0.035200	0.015600	0.000000
8 C	0.152300	0.014500	0.000000
9 C	0.337000	0.015900	0.000000
10 C	0.399100	0.015900	0.000000
11 C	0.900300	0.015100	0.000000
12 C	0.963800	0.016800	0.000000
13 C	0.074600	0.019500	0.000000
14 C	0.136300	0.019400	0.000000
15 C	0.256800	0.019500	0.000000
16 C	0.320100	0.020200	0.000000
17 C	0.882900	0.021300	0.000000
18 C	0.179000	0.020400	0.000000
19 C	0.240800	0.022900	0.000000
20 C	0.525400	0.018600	0.000000
21 C	0.059600	0.024700	0.000000
22 C	0.930500	0.023200	0.000000

unit cell volume (Å³) density (g/cm³) space group elemental ratio - C elemental ratio - Si



SAVE & EXIT

Connecting Experiment and Theory

Extract and store atomic structures

Home > Utkarsh Pratiush > Materials - C_Si_32 (modified by admin)

C_Si_32 (modified by admin)
formula Si₁₆C₁₅₇₃ lattice TET

Description Select Material Actions SAVE & EXIT

Lattice

TET

a	96.000
b	96.000
c	10.000
α	90.000
β	90.000
γ	90.000

Basis

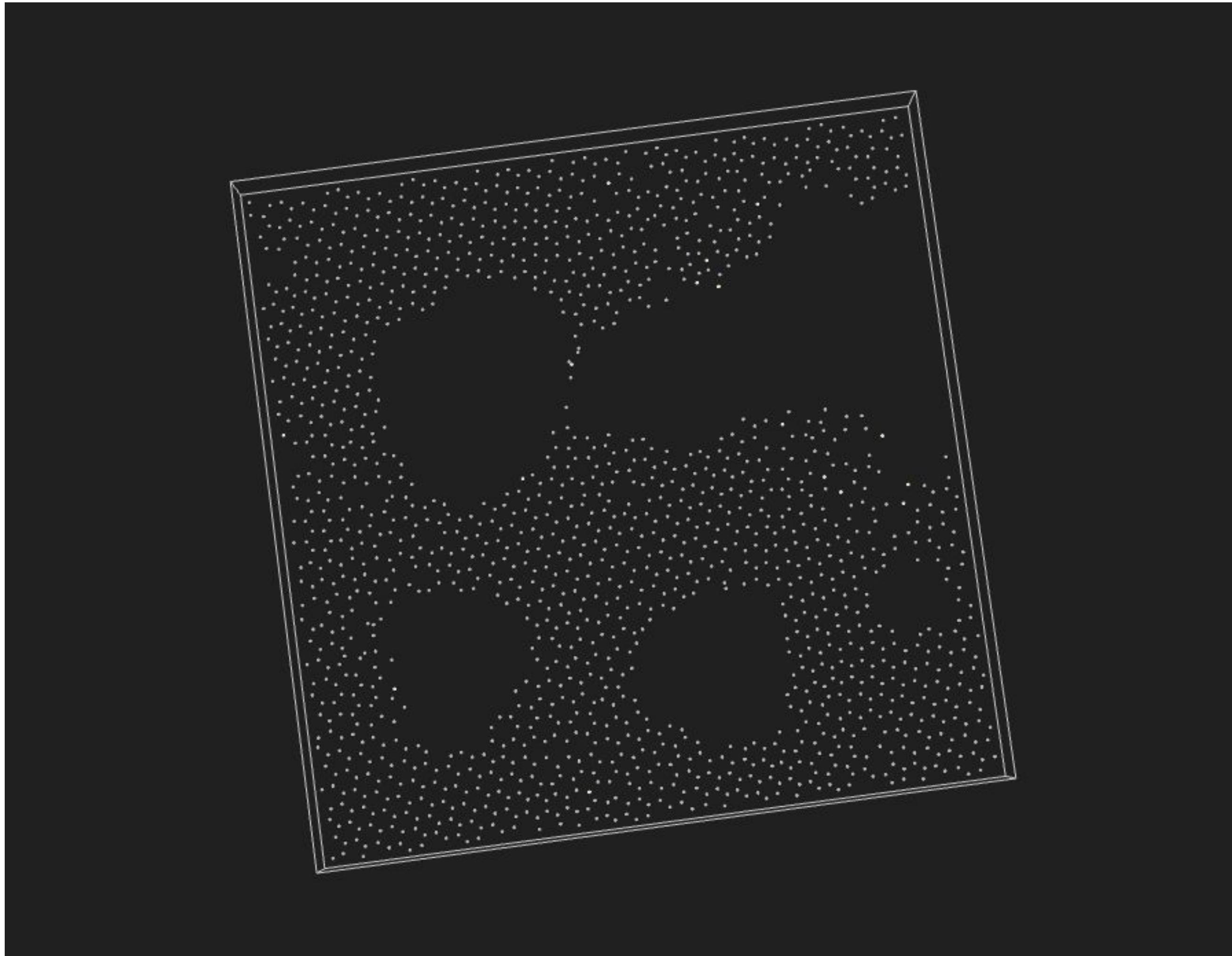
1	C	0.208000	0.010200	0.000000
2	C	0.030300	0.011200	0.000000
3	C	0.073200	0.011700	0.000000
4	C	0.149900	0.010500	0.000000
5	C	0.414100	0.011700	0.000000
6	C	0.332000	0.014200	0.000000
7	C	0.132900	0.015400	0.000000
8	C	0.252900	0.014600	0.000000
9	C	0.395900	0.016000	0.000000
10	C	0.958000	0.015600	0.000000
11	C	0.055700	0.018000	0.000000
12	C	0.177700	0.018300	0.000000
13	C	0.235800	0.017400	0.000000
14	C	0.314900	0.018300	0.000000
15	C	0.898000	0.017600	0.000000
16	C	0.443500	0.019400	0.000000
17	C	0.474400	0.019300	0.000000
18	C	0.881200	0.020400	0.000000
19	C	0.985400	0.021200	0.000000
20	C	0.101000	0.022800	0.000000
21	C	0.162100	0.023400	0.000000
22	C	0.363300	0.023400	0.000000

unit cell volume (Å³) density (g/cm³) space group elemental ratio - C elemental ratio - Si

SAVE & EXIT

Connecting Experiment and Theory

Visualize and inspect structures



Connecting Experiment and Theory

Visualize and inspect structures

The screenshot shows the Mat3ra Materials Designer interface. At the top, there are three tabs: "Mat3ra - Materials R&D Cloud", "C_SI_01 (Modified by admin)", and "Materials Designer". The main window has a dark theme with a purple header bar.

The left sidebar contains a project tree with "C_SI_32" selected, and a formula "Si16C1573" listed. The main area is divided into two sections:

- Crystal Lattice**: This section includes dropdowns for "Lattice units" (angstrom) and "Lattice type" (Tetragonal). It also contains input fields for "Lattice 'a'" (96), "Lattice 'b'" (96), "Lattice 'c'" (10), and angles "angle (b^c)" (90), "angle (a^c)" (90), and "angle (a^b)" (90). A "Scale Interatomic Distances" dropdown is also present. An "APPLY EDITS" button is located at the bottom right of this section.
- Crystal Basis**: This section displays a table of atomic positions. The table has two columns: "CRYSTAL UNITS" and "CARTESIAN UNITS". The "CRYSTAL UNITS" column lists atomic numbers (1-32) and element symbols (C). The "CARTESIAN UNITS" column lists coordinates for each atom. The entire table is scrollable.

To the right of the lattice parameters is a 3D visualization of a tetragonal unit cell. The cell is represented by a wireframe frame containing a grid of small spheres, representing atoms. A coordinate system is shown at the top right of the visualization area.

Connecting Experiment and Theory

Visualize and inspect structures

The screenshot shows the Mat3ra Materials Designer interface. At the top, there are three tabs: "Mat3ra - Materials R&D Cloud", "C_SI_01 (Modified by admin)", and "Materials Designer". The main window has a dark theme with a purple header bar.

The left sidebar contains a project tree with "C_SI_32" selected, and a formula "Si16C1573" listed. The main area is divided into two sections:

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- Crystal Basis**: This section displays a table of atomic positions. The table has two tabs: "CRYSTAL UNITS" and "CARTESIAN UNITS". The "CRYSTAL UNITS" tab shows 32 rows of data, each with a row index (1-32), element symbol (C), and coordinates (x, y, z). The "CARTESIAN UNITS" tab is currently hidden.

To the right of the table is a 3D visualization of a tetragonal unit cell containing a grid of atoms. The visualization includes a coordinate system with red, green, and blue axes. A vertical toolbar on the right side of the visualization panel provides various controls for manipulating the view.

Connecting Experiment and Theory

Organize and search structures

Home > Utkarsh Pratiush

Utkarsh Pratiush
utkarsh
description: Joined on Jan 29, 2023

BIO PROJECTS MATERIALS PROPERTIES WORKFLOWS JOBS

Advanced

Name	Formula	Unit Cell Fc	Actions			
C_Si_32	Si16C1573	Si16 C1573	⋮			
C_Si_32 (modified by admin)	Si16C1573	Si16 C1573	⋮			
C_Si_20	Si13C903	Si26 C1806	⋮			
C_Si_43	Si19C1426	Si19 C1426	⋮			
C_Si_16	Si11C914	Si22 C1828	⋮			
C_Si_08	Si11C976	Si22 C1952	⋮			
C_Si_04	Si23C1975	Si23 C1975	TET	Pm	05-05-202...	⋮
C_Si_41	Si19C1428	Si19 C1428	TET	Pm	05-05-202...	⋮

ADVANCED PRO

AND OR + RULE + GROUP

formula = Si16C1673

name contains

APPLY CLEAR SAVE SEARCH

Rows per page: 100 1–61 of 61 < >

Connecting Experiment and Theory

Organize and search structures

Home > Utkarsh Pratiush

Utkarsh Pratiush
utkarsh
description:Joined on Jan 29, 2023

BIO PROJECTS MATERIALS PROPERTIES WORKFLOWS JOBS

Advanced

Name	Formula	Unit Cell Fc	Actions				
C_Si_32	Si16C1573	Si16 C1573	Si13C903	Si26 C1806	Si19C1426	Si19 C1426	⋮
C_Si_32 (modified by admin)	Si16C1573	Si16 C1573	Si11C914	Si22 C1828	TET	Pm	⋮
C_Si_20	Si13C903	Si26 C1806	Si11C914	Si22 C1828	TET	Pm	⋮
C_Si_43	Si19C1426	Si19 C1426	Si11C914	Si22 C1828	TET	Pm	⋮
C_Si_16	Si19C1426	Si19 C1426	Si11C914	Si22 C1828	TET	Pm	⋮
C_Si_08	Si11C976	Si22 C1952	Si11C976	Si22 C1952	TET	Pm	⋮
C_Si_04	Si23C1975	Si23 C1975	Si23C1975	Si23 C1975	TET	Pm	⋮
C_Si_41	Si19C1428	Si19 C1428	Si19C1428	Si19 C1428	TET	Pm	⋮

const queryObject =
1 v {
2 "createdAt": {"\$gt": "2025-05-21 18:00:00.000"}
3 }
db.collection(materials).find(queryObject)

ADVANCED PRO APPLY CLEAR SAVE SEARCH

Rows per page: 100 1-61 of 61 < >

Connecting Experiment and Theory

Organize and search structures

Home > Utkarsh Pratiush

Utkarsh Pratiush
utkarsh
description: Joined on Jan 29, 2023

BIO PROJECTS MATERIALS PROPERTIES WORKFLOWS JOBS

Advanced

Save search

Example Search

SAVE

Name	Formula	Unit	Actions			
C_Si_32	Si16C1573	Si16	⋮			
C_Si_32 (modified by admin)	Si16C1573	Si16	⋮			
C_Si_20	Si13C903	Si26	⋮			
C_Si_43	Si19C1426	Si19	⋮			
C_Si_16	Si11C914	Si22 C1828	TET	Pm	05-05-202...	⋮
C_Si_08	Si11C976	Si22 C1952	TET	Pm	05-05-202...	⋮
C_Si_04	Si23C1975	Si23 C1975	TET	Pm	05-05-202...	⋮
C_Si_41	Si19C1428	Si19 C1428	TET	Pm	05-05-202...	⋮

Rows per page: 100 1-61 of 61 < >

Connecting Experiment and Theory

Easily Setup and Run Simulation

Home > Workflows Bank

curators

ENTIRE COLLECTION Advanced + Create

Name	Used applic...	Application ...	Subworkflo...	Tags	Created	Account	Creator	Actions
variable-c...	vasp	5.3.0			11-03-201...	curators	exadmin	⋮
Density of ...	vasp	5.3.5	Density o...		11-03-201...	curators	exadmin	⋮
Band Stru...	vasp	5.3.5	Band Stru...		11-03-201...	curators	exadmin	⋮
Band Gap	vasp	5.3.5	Band Gap		11-03-201...	curators	exadmin	⋮
Band Stru...	vasp	5.3.5	Band Stru...		11-03-201...	curators	exadmin	⋮
Total Ener...	vasp	5.3.5	Total Ener...		11-03-201...	curators	exadmin	⋮
K-point Co...	espresso	6.3	K-point C...		11-03-201...	curators	exadmin	⋮
Zero Point ...	espresso	6.3	Zero Poin...		11-03-201...	curators	exadmin	⋮
Recalculat...	espresso	6.3	Recalcula...		11-03-201...	curators	exadmin	⋮
Electronic ...	espresso	6.3	Electronic...		11-03-201...	curators	exadmin	⋮
Fixed-cell ...	espresso	6.3	Fixed-cell ...		11-03-201...	curators	exadmin	⋮
Variable-c...	espresso	6.3	Variable-c...		11-03-201...	curators	exadmin	⋮

Rows per page: 50 ▾ 1-50 of 55 < >

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Platform version 2025.4.24.

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MAT^{ERA}

Connecting Experiment and Theory

Easily Setup and Run Simulation

Home > Utkarsh Pratiush

Utkarsh Pratiush
utkarsh
description: Joined on Jan 29, 2023

BIO PROJECTS MATERIALS 1 PROPERTIES WORKFLOWS JOBS SERVICE LEVELS PREFERENCES

Import + CREATE + SET

ENTIRE COLLECTION Advanced

1 workflow COPY DELETE SHARE MOVE TO SET

Name	Used application	Application Version	Subworkflows	Tags	Default	Up-to-date	Shared	Public	Ext+Ink	Ext+web	Actions
Fixed-cell Relaxation (clone)	espresso	6.3	Fixed-cell Relaxation			✓					
Total Energy	espresso	6.3	Total Energy		✓	✓					

1 row selected Rows per page: 100 1–2 of 2

Connecting Experiment and Theory

Easily Setup and Run Simulation

The screenshot displays the MATERA software interface for managing workflows. The top navigation bar shows the path: Home > Utkarsh Pratiush > Workflows - Fixed-cell Relaxation (clone). The main title is "Fixed-cell Relaxation (clone)" under the "applications espresso" category. On the right, there are buttons for "Description", "Select Workflow Actions", "SAVE & EXIT", and a dropdown menu.

The left panel contains a summary of the workflow, including its name ("Fixed-cell Relaxation"), Flowchart ID ("7f2011b23ae969af1c6d977"), and actions like "COPY" and "DELETE". It also has sections for "OVERVIEW" and "UNITS".

The right panel provides a detailed view of the workflow. It shows the title "Fixed-cell Relaxation espresso" and tabs for "OVERVIEW", "IMPORTANT SETTINGS", "DETAILED VIEW", and "COMPUTE". Below these tabs is a "DETAILS" section. The "UNITS" section lists a single unit named "pw_relax" (Flowchart ID: e09d81b0-a05...), which is highlighted with a blue border. This unit is connected to a "Start" node at the top of a grid-based timeline. The timeline consists of a grid of small squares, likely representing time steps or frames. The "pw_relax" unit is positioned at the bottom of the first column of the grid.

Connecting Experiment and Theory

Easily Setup and Run Simulation

The screenshot shows a Jupyter Notebook interface with two main sections: 'Create jobs' and 'Extract results'. On the left, there is a file browser showing several IPython notebook files. The 'Create jobs' section contains code for creating jobs, moving them to a set, and submitting them. The 'Extract results' section contains code for extracting final structures and band gaps from simulation jobs.

Create jobs

Create jobs for the materials above.

```
[ ]: compute = job_endpoints.get_compute(CLUSTER_NAME, PPN, NODES, QUEUE_NAME, TIME_LIMIT)
jobs = job_endpoints.create_by_ids(materials, workflow_id, project_id, JOB_NAME_PREFIX, OWNER_ID, compute)
```

Create a jobs set and move the jobs into it.

```
[ ]: jobs_set = job_endpoints.create_set({"name": JOBS_SET_NAME, "projectId": project_id, "owner": {"_id": OWNER_ID}})
for job in jobs:
    job_endpoints.move_to_set(job["_id"], "", jobs_set["_id"])
```

Submit the jobs for execution.

```
[ ]: for job in jobs:
    job_endpoints.submit(job["_id"])
```

Monitor the jobs and print the status until they are all finished.

```
[ ]: job_ids = [job["_id"] for job in jobs]
wait_for_jobs_to_finish(job_endpoints, job_ids)
```

Extract results

For each material, simulation job, final structure, pressure and band gaps are extracted.

- Final structure and pressure are extracted from the first unit (vasp_relax with index 0) of the first job's subworkflow (volume-relaxation with index 0)
- Band gaps are extracted from the second unit (vasp-bands with index 1) of the second job's subworkflow (SCF-BS-BG-DOS with index 1).

```
[ ]: results = []
for material in materials:
    job = next((job for job in jobs if job["_material"]["_id"] == material["_id"]))
    final_structure = get_property_by_subworkflow_and_unit_indices(property_endpoints, "final_structure", job, 0, 0)[
        "data"]
```

UPCOMING: STEM-specific functionality

What's Possible when creating a Digital link Exp. <> Theory

Community-driven digital materials R&D ecosystem

- Organize experimental to making it **accessible from anywhere online** and enabling **collaboration/sharing** of the data
- Incorporate Modeling & Simulations approaches and AI/ML techniques to assist with experimental data analysis
- Make decisions on the next course of action based on “theory-in-the-loop”
- Close the loop and automate the process for both theory and experimental workflows

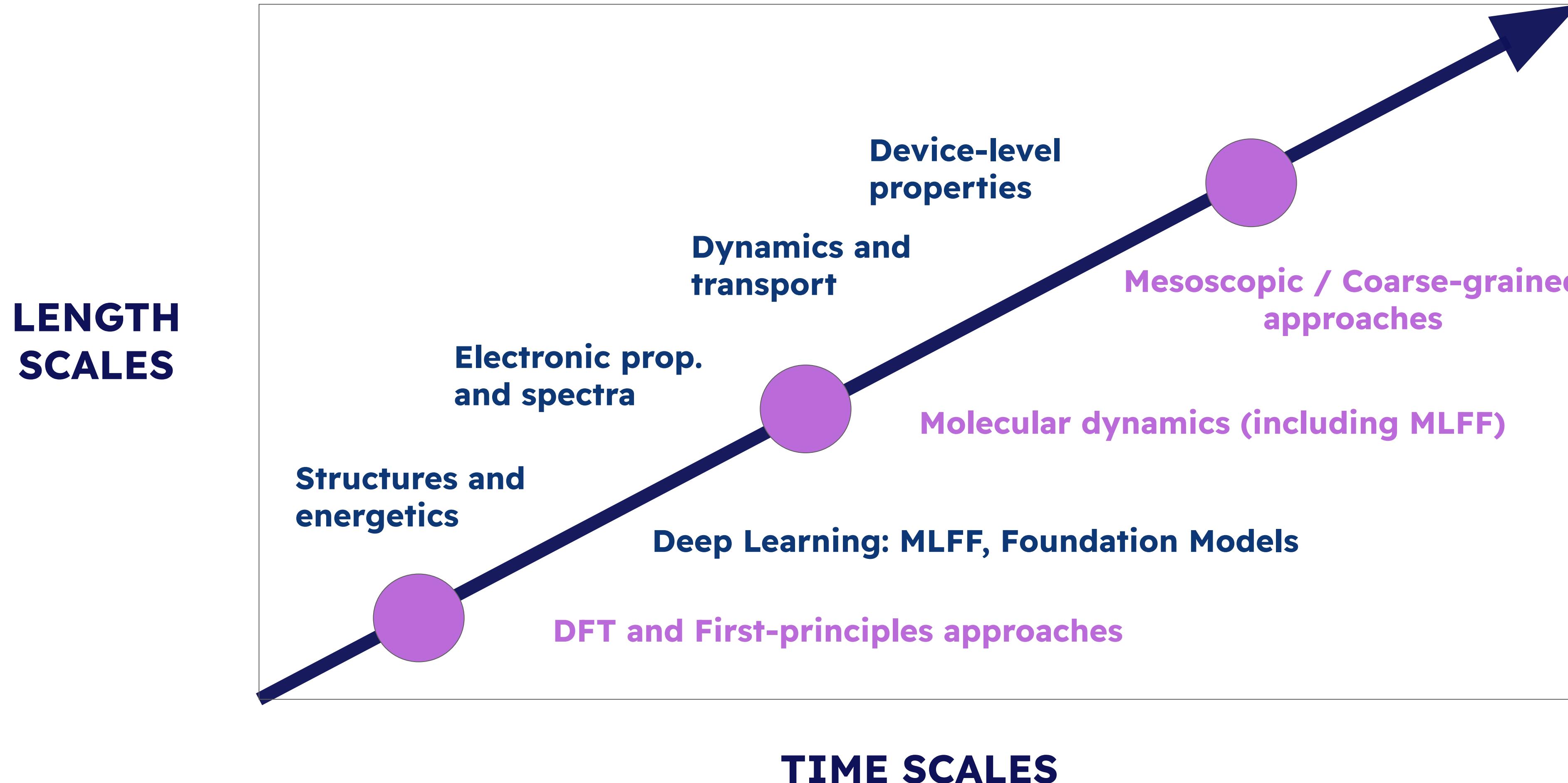
STEM specific M&S, AI/ML Items

Based on preliminary discussions

- Structure reconstruction: via a combination of Molecular Dynamics and/or Foundation Models plus Density Functional Theory
- EELS spectra from DFT
- XRD Spectra from DFT
- Simulated STEM images from DFT
- Closed-loop data exchange
- Active learning
- Automated experimentation

STEM related M&S, AI/ML Items: roadmap

Based on preliminary discussions



Summary

Mat3ra 4 STEM: accelerating materials R&D for nanoscale

- Advances in microelectronics depend on materials, processing, and manufacturing from nanoscale. Mat3ra.com aims to accelerate materials R&D for microelectronics by making advanced simulations and AI/ML **accessible & collaborative**.
- Mat3ra facilitates:(1) **agile** (fast and inexpensive) **deployment of new R&D capability** enabling faster testing and adoption of rapidly developing AI/ML and HPC tools;(2) **collaboration** online at intra- or inter-organizational levels increasing productivity and efficiency.
- Mat3ra.com has started working on integrating and organizing experimental data, and a set of representative use cases for it. Maturing the deployment and including UTK use cases for nano-electronics are planned.



MATERIALS R&D CLOUD

Sign up at:

<https://platform.mat3ra.com/register>

