

Data Standards: the enabler of AI-ready collaborative materials R&D

MAT³RA



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Summary

Join us in building community-driven digital materials R&D ecosystem together

- Mat3ra.com is a **digital ecosystem** accelerating materials R&D by making digital techniques developed by the scientific community accessible & collaborative.
- Our focus is on **modeling and simulations** at the nanoscale (Density Functional Theory, Molecular Dynamics, etc.) and related AI/ML.
- Mat3ra.com has (1) over 10,000 users, and (2) dozens of customers, including AFRL, Merck KGaA, and Shell. This provided a set of learnings resulting in an **open-source data standards** framework described here.
- Join our informal “Social Hour” **5-6p** to learn more and explore collaborative opportunities.

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 |

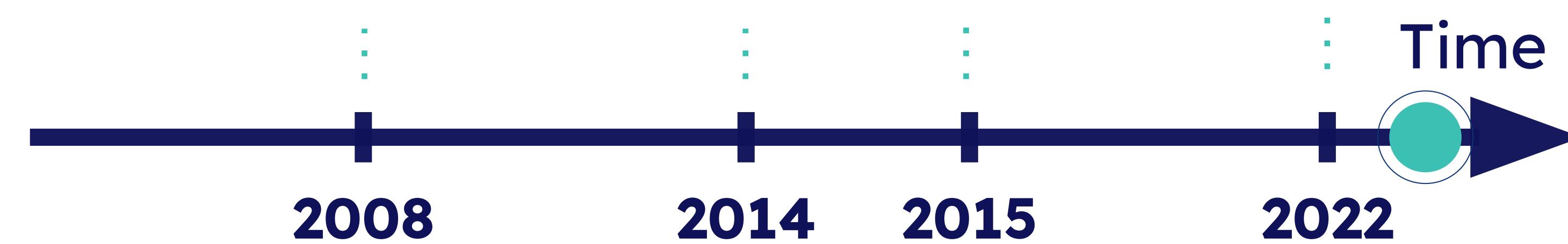
The screenshot shows a news article from The Wall Street Journal. The headline reads "Startup That Models Materials at Atomic Level Raises Seed Capital". Below the headline, there is a section titled "CIO JOURNAL" with the sub-section "MATERIAL". It features a visualization of a molecular structure with atoms labeled with values like 7.7348, 99.2000, 13.758, and 13.468. To the right, there is a sidebar with the Deloitte logo and several smaller headlines related to technology and innovation.

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

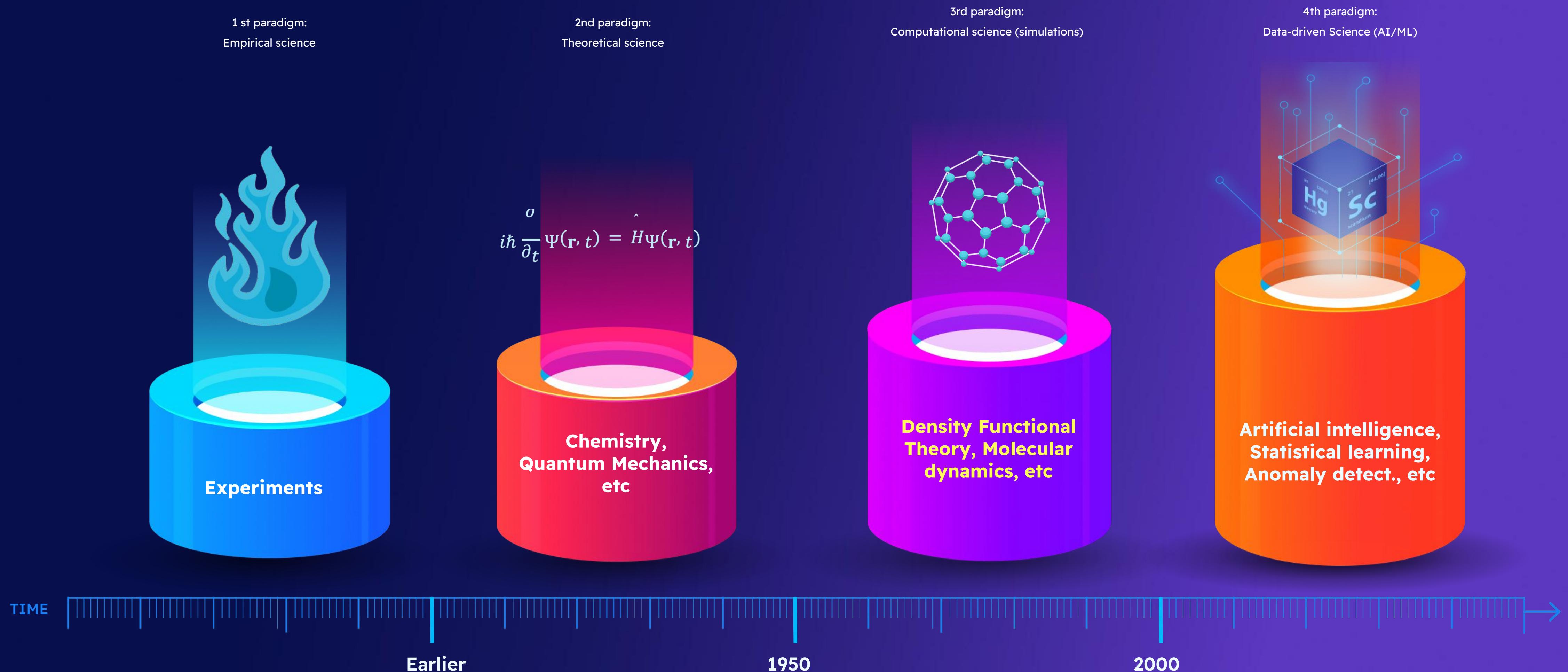
Mat3ra.com emerged
as a successor
of Exabyte.io



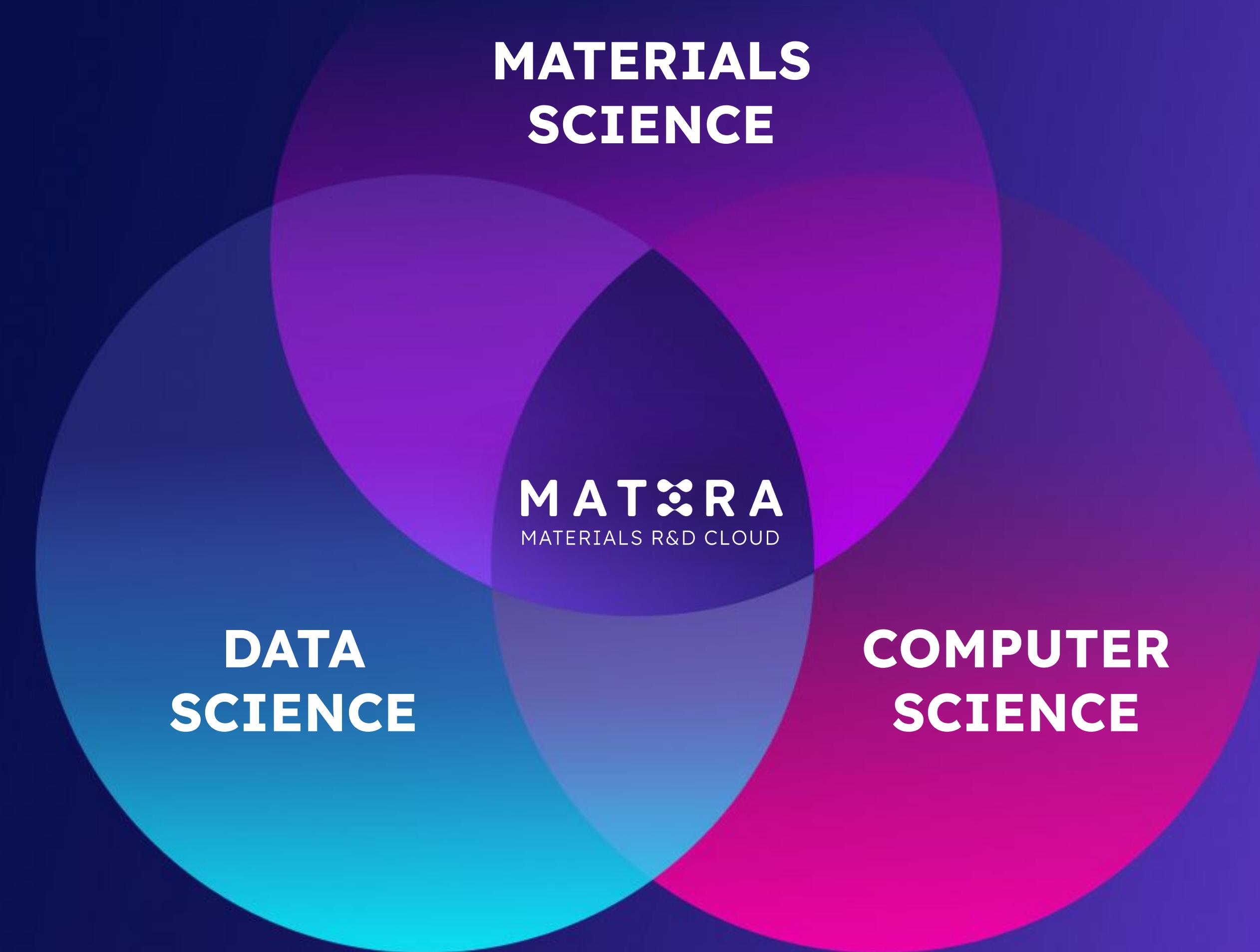
INTRODUCTION

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

The Company

Accelerate Materials R&D through widespread adoption of digital tools

- Founded 2015 out of UC Berkeley
- \$3.8M in VC funding (incl. Peter Thiel, Tim Draper)
- \$3.5M in Gov funding (AFVentures/AFWERX, DoE, DoC/NIST)
- HQ in USA, presence in Japan, India
- Users at hundreds of universities, dozens of Global 2000 customers

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

70,000+

CALCULATIONS
RUN

40,000+

MATERIALS
STORED

10,000+

SCIENTISTS
WORLDWIDE

300+

UNIVERSITIES

20+

ENTERPRISE
CUSTOMERS

Our Customers

Global presence with long-term enterprise and public sector customer relationships

TRUSTED BY



'TORAY'



ITOCHU

Asahi KASEI

KYOCERA



DENSO



NIPPON
CHEMI-CON

2024-07-18: Why are we here?

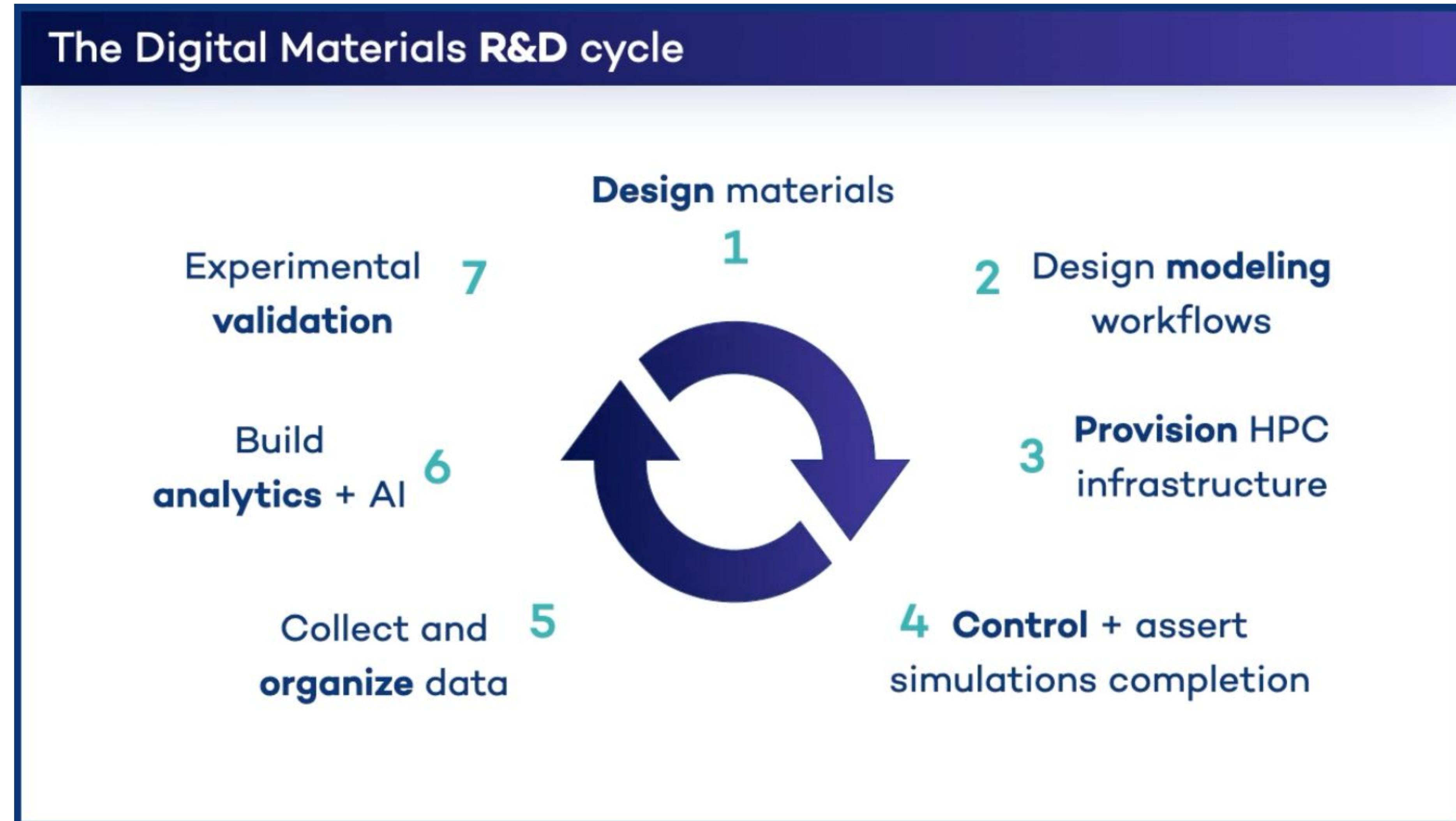
To promote community-wide collaboration and provide an avenue for commercialization



THE MAT3RA PLATFORM

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

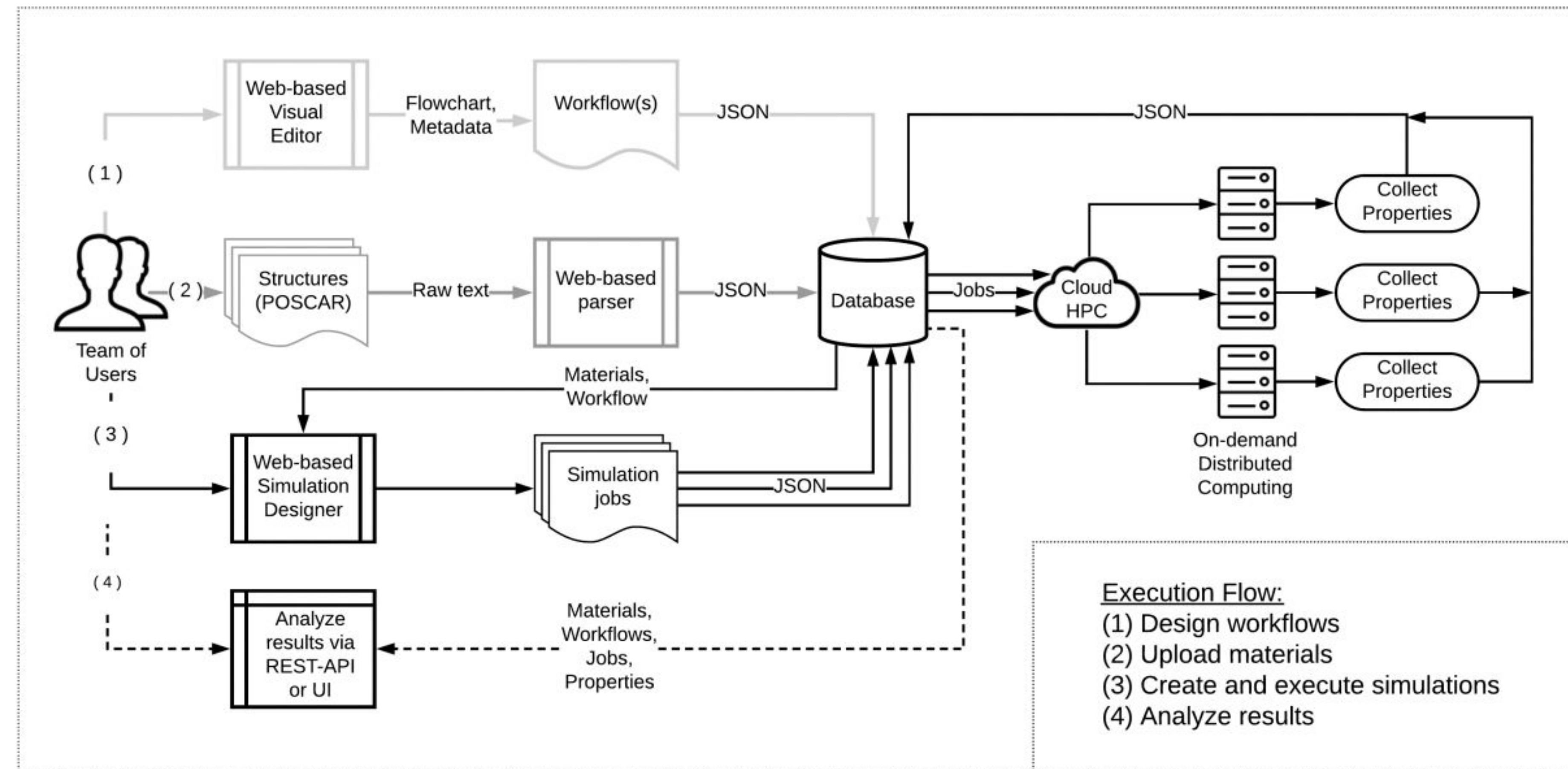
AI-ready, well-organized structured data. Support for multiple R&D activities. Agile digital practices.



MAT[∞]RA
MATERIALS R&D CLOUD

Simulation execution flow

Declarative approach versed in static searchable data (JSON) instead of scripts and/or code only



THE APPROACH

OPEN-SOURCE, DATA-CENTRIC

Our approach to organizing Materials R&D

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

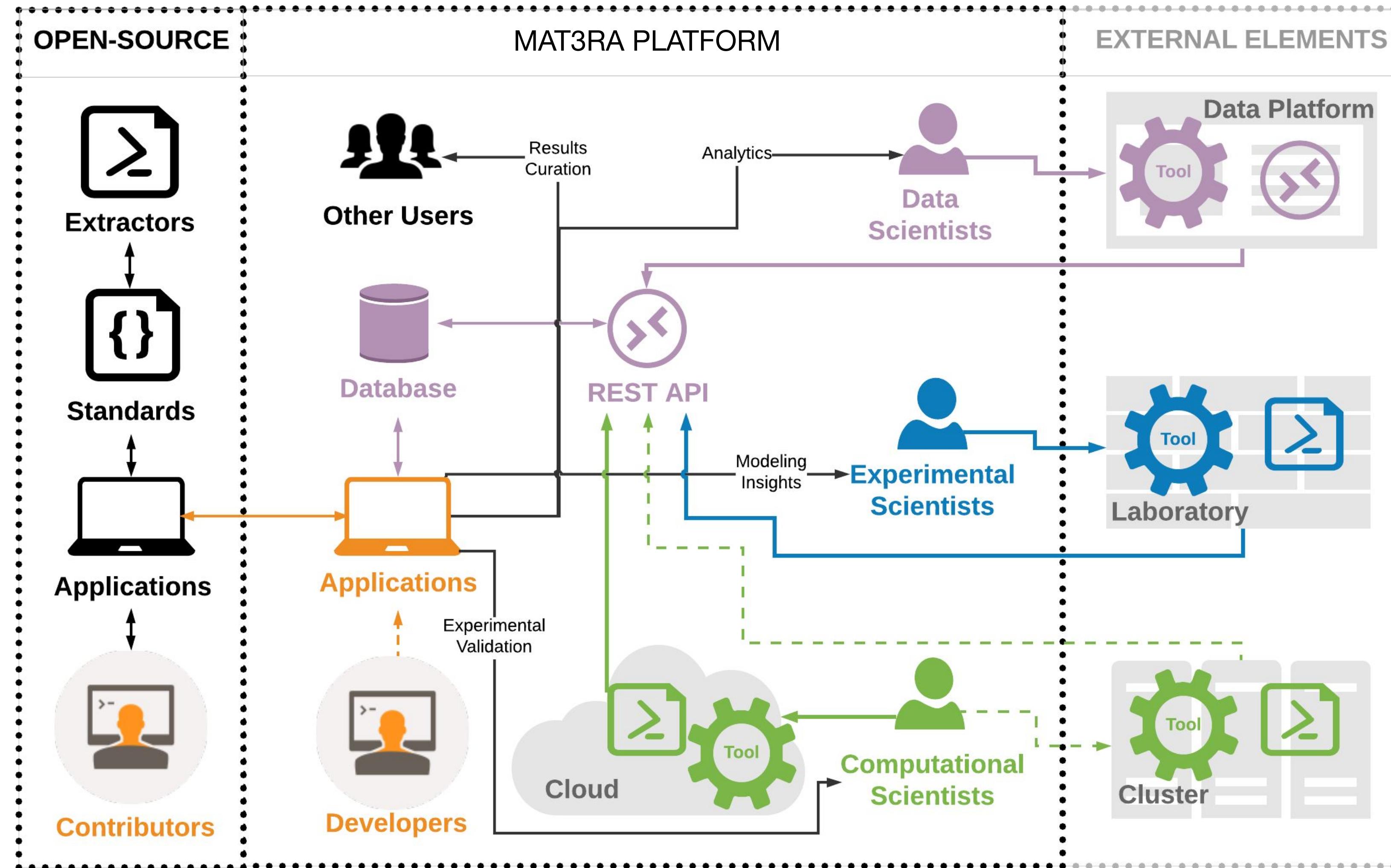
The screenshot shows the GitHub organization page for Mat3ra.com. The top navigation bar includes the GitHub logo, a search bar, and links for Pull requests, Issues, Trending, and Explore. The organization profile card for Mat3ra.com displays a verified badge, 34 followers, location in San Francisco, 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'.

Our approach to organizing Materials R&D

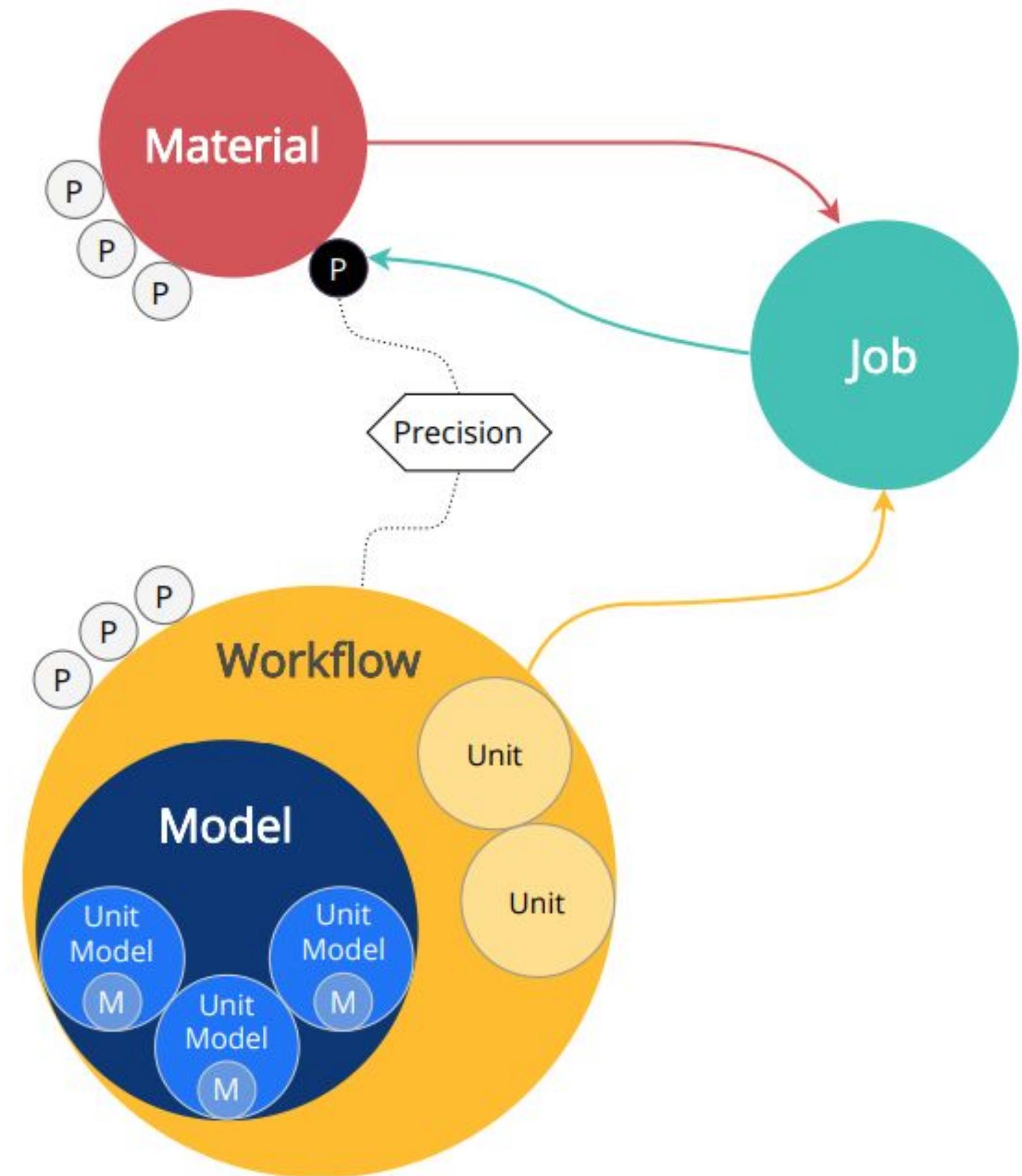
(1) Open-source code, (2) community-driven data, (3) inclusive design for new apps/compute/data



- 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

Data Standards (1) ontology

Entities and their relationship



Data Standards (1) ontology

Entities and their relationship

| <u>Domain</u> | <u>Workflow Logic</u> | <u>Application Used</u> | <u>Model Approach</u> | <u>Material ID</u> | <u>Property Extracted</u> | <u>Infrastructure Used</u> |
|---------------|-----------------------|-------------------------|-----------------------|--------------------|---------------------------|----------------------------|
| | Workflow | Application | Model | Material | RawProperty | Cluster |
| | Subworkflow | Executable | Method | Molecule | RefinedProperty | Node |
| | Unit | Flavor | MethodData | | BestProperty | Queue |
| | ContextProvider | Template | | | ProtoProperty | Job |
| | | | | | MetaProperty | |

Data Standards (1) ontology

Entities and their relationship

| Domain | <u>Computational</u> | <u>Experimental</u> | <u>Data</u> | <u>Developer</u> | <u>Curator</u> |
|--------|----------------------|---------------------|-------------|-----------------------|----------------|
| | Expert Scientist | Scientist | Scientist | Application Developer | Regular User |
| | Novice Scientist | | Engineer | | Data Curator |

Data Standards (2): categories

Entity types categorization: example Model Categories

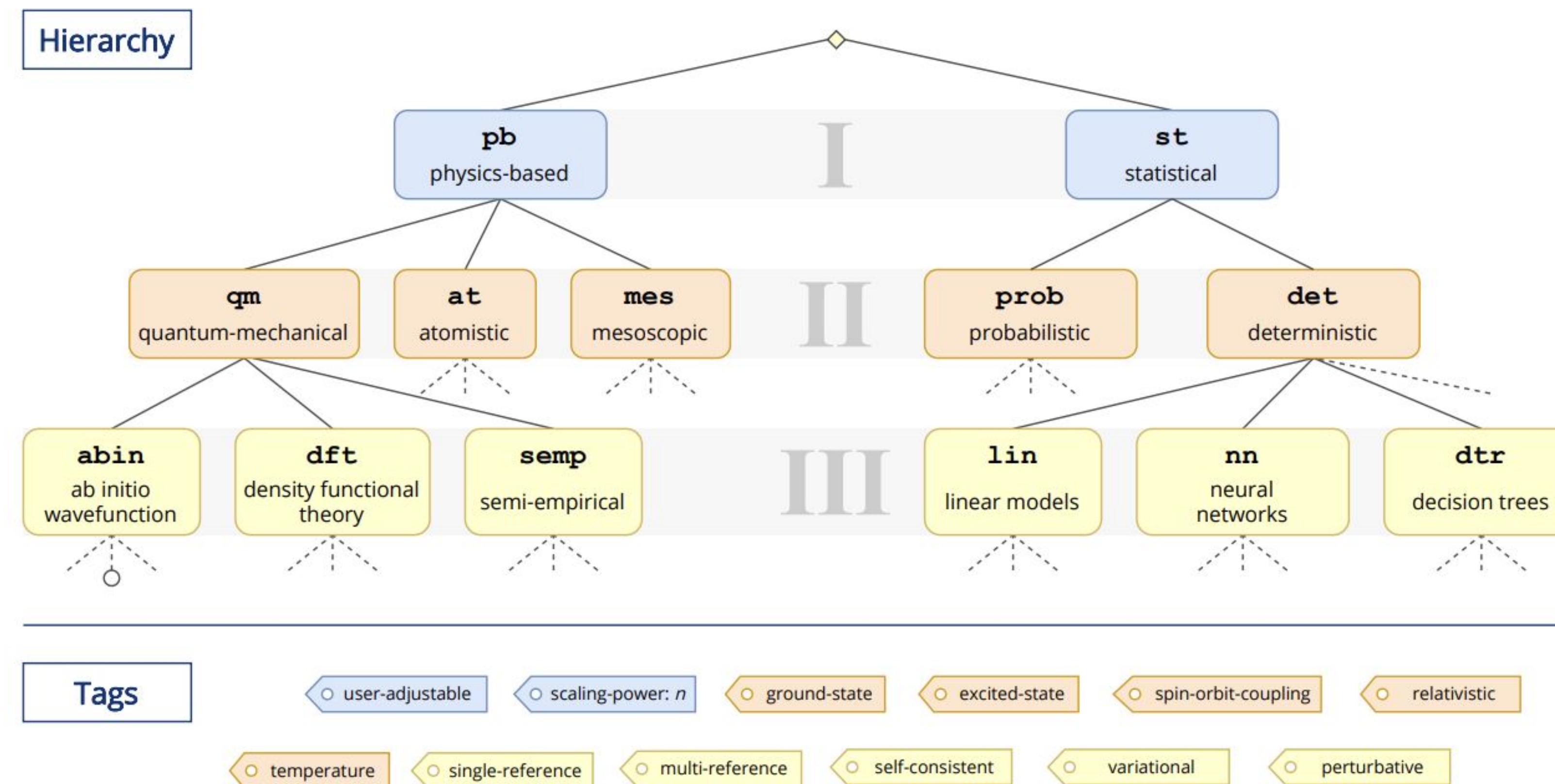


Figure 2: Schematic representation of the tiers of the CateCom categorization. Tier I to tier III of the unit model classification hierarchy and descriptive tags colored according to the tier in which they first appear.

Data Standards (2): categories

Entity types categorization: example Material Categories

Click to go forward, hold to see history <https://github.com/Exabyte-io/standata/blob/main/materials/categories.yml>

Files

- main
- +
- Go to file
- TiO2-[Titanium_Oxide]-TET_[P4...]
- VO2-[Vanadium_IV_Oxide]-TET_...
- WS2-[Tungsten_Disulfide]-HEX...
- WS2-[Tungsten_Disulfide]-HEX...
- WSe2-[Tungsten_Diselenide]-H...
- WSe2-[Tungsten_Diselenide]-H...
- Y2O3-[Yttrium_III_Oxide]-MCLC...
- Y2O3-[Yttrium_III_Oxide]-MCL...
- ZnO-[Zinc_Oxide]-HEX_[P6_3m...
- ZrO2-[Zirconium_Dioxide]-MCL...
- categories.yml
- properties
- src
- tests
- workflows
- .babelrc
- .eslintrc.json
- .gitignore
- .mocharc.json
- .nycrc

Code Blame 234 lines (233 loc) · 5.37 KB

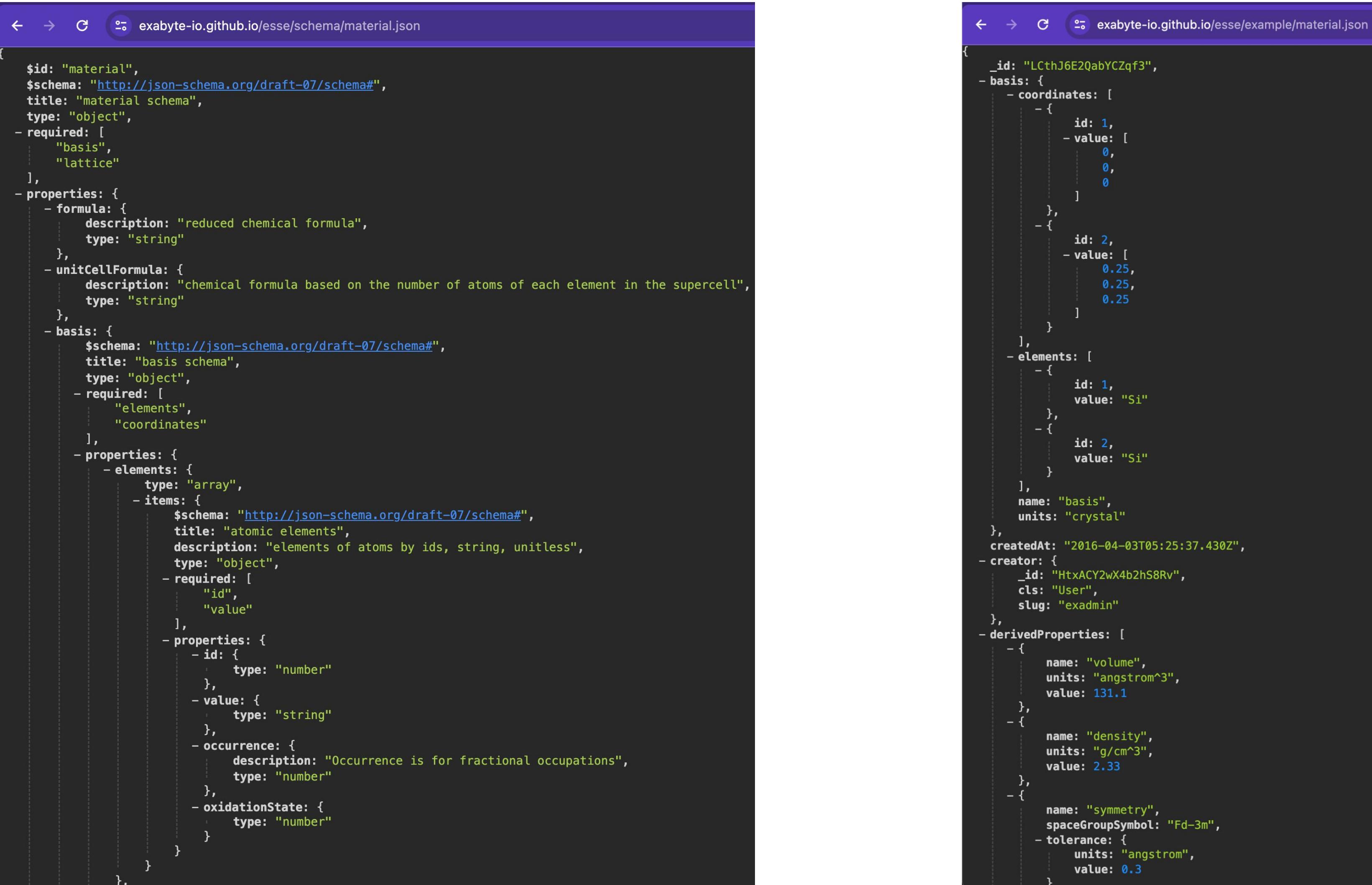
```
1 categories:
2   type:
3     - semiconductor
4     - solar energy material
5     - storage medium
6     - organic electronics
7     - battery/energy storage
8     - composite
9     - polymer
10    - metals & alloys
11    - solvent
12    - catalysis
13    - consumer packaged goods
14    - glass
15    - ceramic
16    form_factor:
17      - bulk
18      - layer
19      - interface
20    dimensionality:
21      - 0D
22      - 1D
23      - 2D
24      - 3D
25      - 4D
26    electrical_conductivity:
27      - metal
28      - semi-metal
29      - semiconductor
30      - insulator
31    magnetism:
32      - ferromagnetic
33      - anti-ferromagnetic
34      - paramagnetic
35      - diamagnetic
36      - non-magnetic
```

Code Blame 49 lines (48 loc) · 943 Bytes

```
1 categories:
2   type:
3     - mechanical
4     - electronic
5     - magnetic
6     - thermal
7     - optical
8     - dynamic
9     - transport
10    - radiological
11    - acoustic
12    - manufacturing
13    - chemical
14    - structural
15    - surface
16    property_class:
17      - meta-property
18      - proto-property
19    value_type:
20      - scalar
21      - vector
22      - matrix
23      - tensor_rank3
24      - tensor_rank4
25      - non-scalar
26    measurement:
27      - angle-resolved-photoemission-spectroscopy
28      - atomic-force-microscopy
29      - x-ray-diffraction
30      - x-ray-fluorescence
31      - transmission-electron-microscopy
32      - scanning-electron-microscopy
33      - thermogravimetric-analysis
34    application:
35      - espresso
36      - vasp
```

Data Standards (3): schemas and examples (+community)

Entity schema - left - and example - right



The image shows two side-by-side code editors displaying JSON documents. The left editor contains the 'material.json' schema, and the right editor contains an example document named 'material.json'. Both are hosted on the URL <https://exabyte-io.github.io/esse/>.

Entity schema - material.json

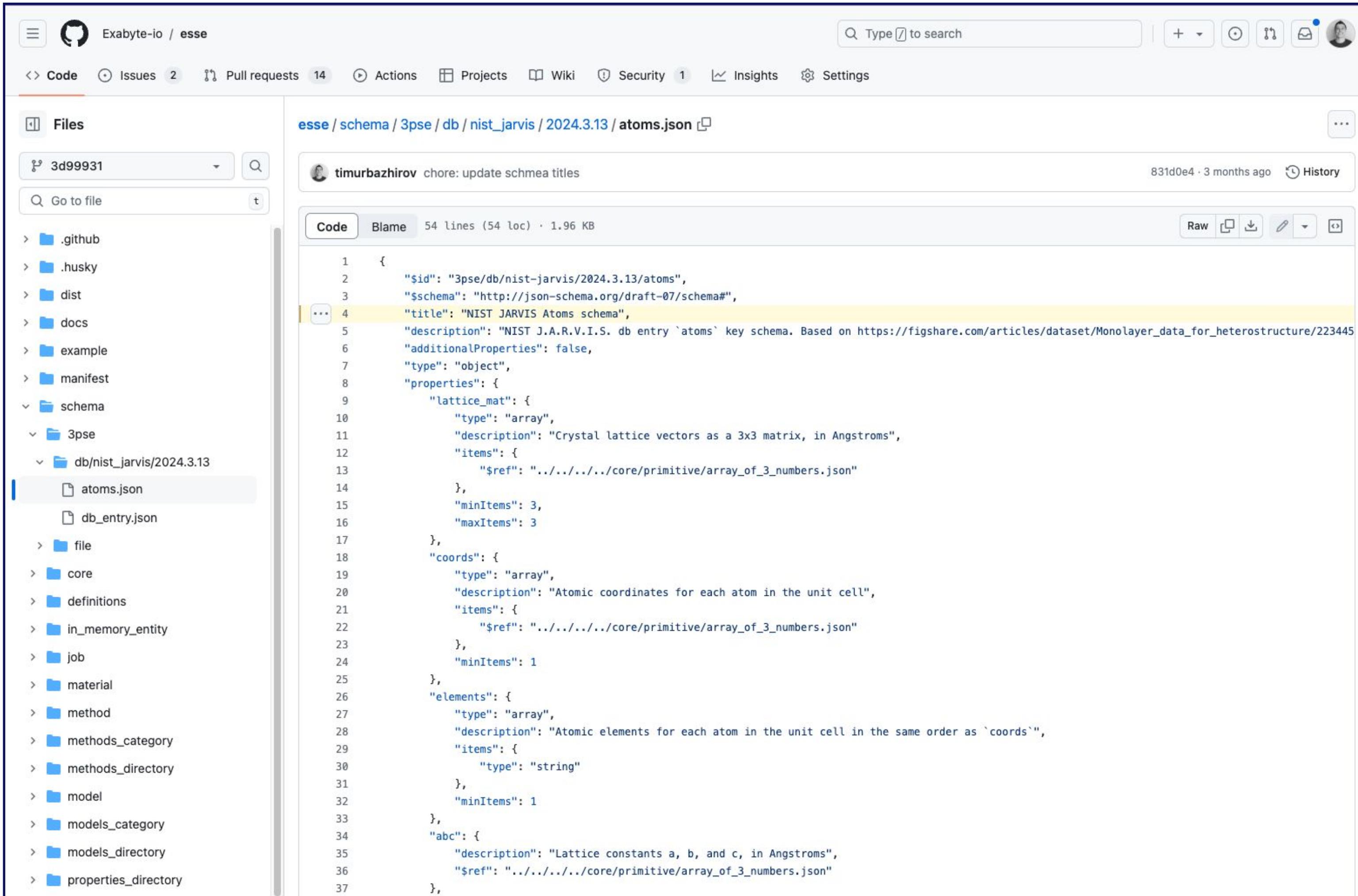
```
{
  "$id": "material",
  "$schema": "http://json-schema.org/draft-07/schema#",
  "title": "material schema",
  "type": "object",
  "- required: [
    "basis",
    "lattice"
  ],
  "- properties: {
    - formula: {
      description: "reduced chemical formula",
      type: "string"
    },
    - unitCellFormula: {
      description: "chemical formula based on the number of atoms of each element in the supercell",
      type: "string"
    },
    - basis: {
      $schema: "http://json-schema.org/draft-07/schema#",
      title: "basis schema",
      type: "object",
      - required: [
        "elements",
        "coordinates"
      ],
      - properties: {
        - elements: {
          type: "array",
          - items: {
            $schema: "http://json-schema.org/draft-07/schema#",
            title: "atomic elements",
            description: "elements of atoms by ids, string, unitless",
            type: "object",
            - required: [
              "id",
              "value"
            ],
            - properties: {
              - id: {
                type: "number"
              },
              - value: {
                type: "string"
              },
              - occurrence: {
                description: "Occurrence is for fractional occupations",
                type: "number"
              },
              - oxidationState: {
                type: "number"
              }
            }
          }
        }
      }
    }
  }
}
```

Example - material.json

```
{
  "_id": "LCtthJ6E2QabYCZqf3",
  "- basis: {
    - coordinates: [
      - {
        id: 1,
        - value: [
          0,
          0,
          0
        ]
      },
      - {
        id: 2,
        - value: [
          0.25,
          0.25,
          0.25
        ]
      }
    ],
    - elements: [
      - {
        id: 1,
        value: "Si"
      },
      - {
        id: 2,
        value: "Si"
      }
    ],
    name: "basis",
    units: "crystal"
  },
  createdAt: "2016-04-03T05:25:37.430Z",
  - creator: {
    _id: "HtxACY2wX4b2hS8Rv",
    cls: "User",
    slug: "exadmin"
  },
  - derivedProperties: [
    - {
      name: "volume",
      units: "angstrom^3",
      value: 131.1
    },
    - {
      name: "density",
      units: "g/cm^3",
      value: 2.33
    },
    - {
      name: "symmetry",
      spaceGroupSymbol: "Fd-3m",
      - tolerance: {
        units: "angstrom",
        value: 0.3
      }
    }
  ]
}
```

Data Standards (3): schemas and examples (+community)

Entity schema for JARVIS NIST db entry Atoms

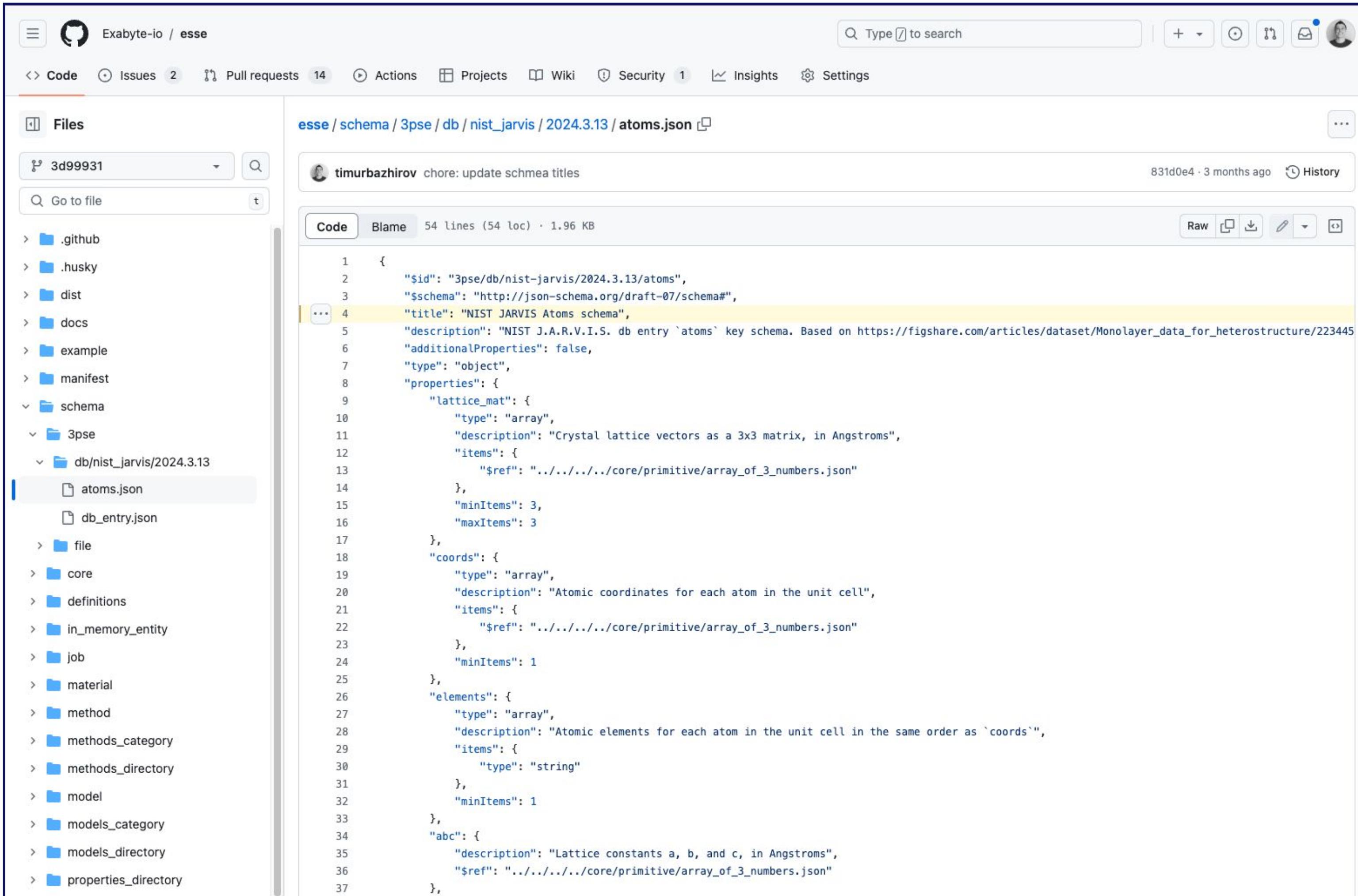


The screenshot shows a GitHub repository interface for the 'esse' project. The repository path is `esse / schema / 3pse / db / nist_jarvis / 2024.3.13 / atoms.json`. The file was last updated by `timurbazhirov` on `chore: update schmea titles` at `831d0e4 · 3 months ago`. The code editor displays the JSON schema for the 'Atoms' entity. The schema defines properties for 'lattice_mat', 'coords', 'elements', and 'abc'. It includes descriptions and \$ref links to other schema files.

```
1  {
2    "$id": "3pse/db/nist-jarvis/2024.3.13/atoms",
3    "$schema": "http://json-schema.org/draft-07/schema#",
4    "title": "NIST JARVIS Atoms schema",
5    "description": "NIST J.A.R.V.I.S. db entry `atoms` key schema. Based on https://figshare.com/articles/dataset/Monolayer_data_for_heterostructure/223445",
6    "additionalProperties": false,
7    "type": "object",
8    "properties": {
9      "lattice_mat": {
10        "type": "array",
11        "description": "Crystal lattice vectors as a 3x3 matrix, in Angstroms",
12        "items": {
13          "$ref": "../../../../core/primitive/array_of_3_numbers.json"
14        },
15        "minItems": 3,
16        "maxItems": 3
17      },
18      "coords": {
19        "type": "array",
20        "description": "Atomic coordinates for each atom in the unit cell",
21        "items": {
22          "$ref": "../../../../core/primitive/array_of_3_numbers.json"
23        },
24        "minItems": 1
25      },
26      "elements": {
27        "type": "array",
28        "description": "Atomic elements for each atom in the unit cell in the same order as `coords`",
29        "items": {
30          "type": "string"
31        },
32        "minItems": 1
33      },
34      "abc": {
35        "description": "Lattice constants a, b, and c, in Angstroms",
36        "$ref": "../../../../core/primitive/array_of_3_numbers.json"
37      }
38    }
39  }
```

Data Standards (3): schemas and examples (+community)

Entity schema for JARVIS NIST db entry Atoms



The screenshot shows a GitHub repository interface for the 'esse' project. The repository path is `esse / schema / 3pse / db / nist_jarvis / 2024.3.13 / atoms.json`. The file was last updated by `timurbazhirov` on `chore: update schmea titles` at `831d0e4 · 3 months ago`.

The code editor displays the JSON schema for the 'Atoms' entity. The schema defines the structure of a crystal lattice with properties for lattice vectors, atomic coordinates, elements, and lattice constants.

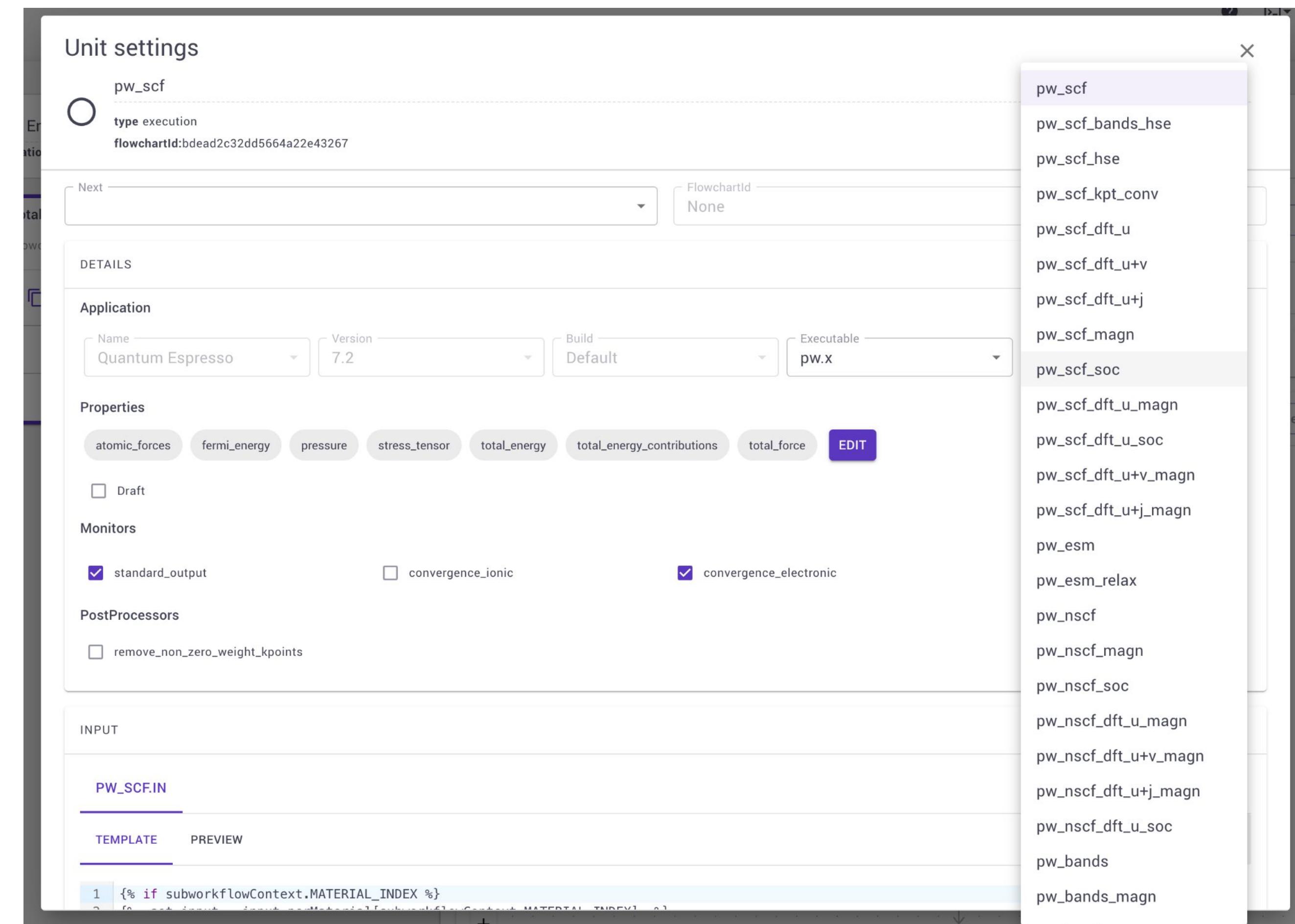
```
1  {
2    "$id": "3pse/db/nist-jarvis/2024.3.13/atoms",
3    "$schema": "http://json-schema.org/draft-07/schema#",
4    "title": "NIST JARVIS Atoms schema",
5    "description": "NIST J.A.R.V.I.S. db entry `atoms` key schema. Based on https://figshare.com/articles/dataset/Monolayer_data_for_heterostructure/223445",
6    "additionalProperties": false,
7    "type": "object",
8    "properties": {
9      "lattice_mat": {
10        "type": "array",
11        "description": "Crystal lattice vectors as a 3x3 matrix, in Angstroms",
12        "items": {
13          "$ref": "../../../../core/primitive/array_of_3_numbers.json"
14        },
15        "minItems": 3,
16        "maxItems": 3
17      },
18      "coords": {
19        "type": "array",
20        "description": "Atomic coordinates for each atom in the unit cell",
21        "items": {
22          "$ref": "../../../../core/primitive/array_of_3_numbers.json"
23        },
24        "minItems": 1
25      },
26      "elements": {
27        "type": "array",
28        "description": "Atomic elements for each atom in the unit cell in the same order as `coords`",
29        "items": {
30          "type": "string"
31        },
32        "minItems": 1
33      },
34      "abc": {
35        "description": "Lattice constants a, b, and c, in Angstroms",
36        "$ref": "../../../../core/primitive/array_of_3_numbers.json"
37      }
38    }
39  }
```

Community contributions: (1) default workflows “LEGOs”

Platform users modify the default workflows to create new ones.

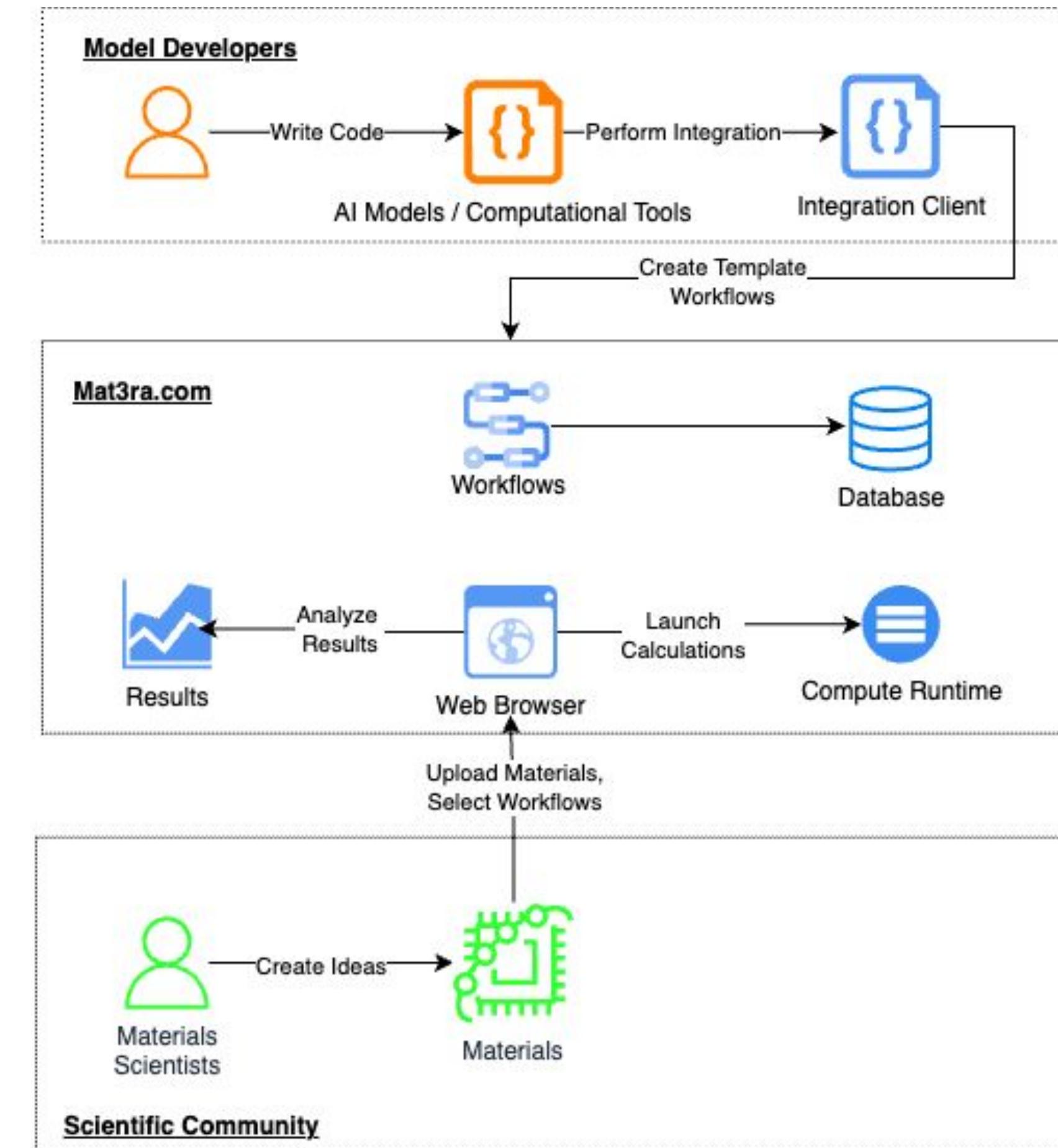
A screenshot of a GitHub repository page for the 'Exabyte-io / wode.js' repository. The URL in the address bar is github.com/Exabyte-io/wode.js/blob/main/assets/subworkflows/espresso/band_gap_hse_dos.yml. The repository has 1 issue and 7 pull requests. The 'Code' tab is selected. On the left, there's a sidebar with 'Files' and a tree view of files under 'assets'. The main area shows the content of 'band_gap_hse_dos.yml':

```
1 name: HSE Band Gap
2 application:
3   name: espresso
4   version: "6.3"
5   model:
6     name: DFTModel
7     config:
8       type: dft
9       subtype: hybrid
10      functional:
11        name: hse06
12        slug: hse06
13      method:
14        name: PseudopotentialMethod
15        config:
16          type: pseudopotential
17          subtype: us
18        units:
19          - config:
20            execName: pw.x
21            flavorName: pw_scf_hse
22            name: pw_scf_hse
23            functions:
24              head: true
25              type: executionBuilder
26            - config:
27              execName: projwfc.x
28              flavorName: projwfc
29              name: projwfc
30              type: executionBuilder
```



Community contributions: (2) custom apps, workflows

Code developers can contribute to the platform to provide improved UX for all platform audience.



USE CASES

HOW THE PLATFORM IS USED

Representative Case Studies

Representative case studies demonstrating what's possible today.

1. Semiconductor / Electronic Materials

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

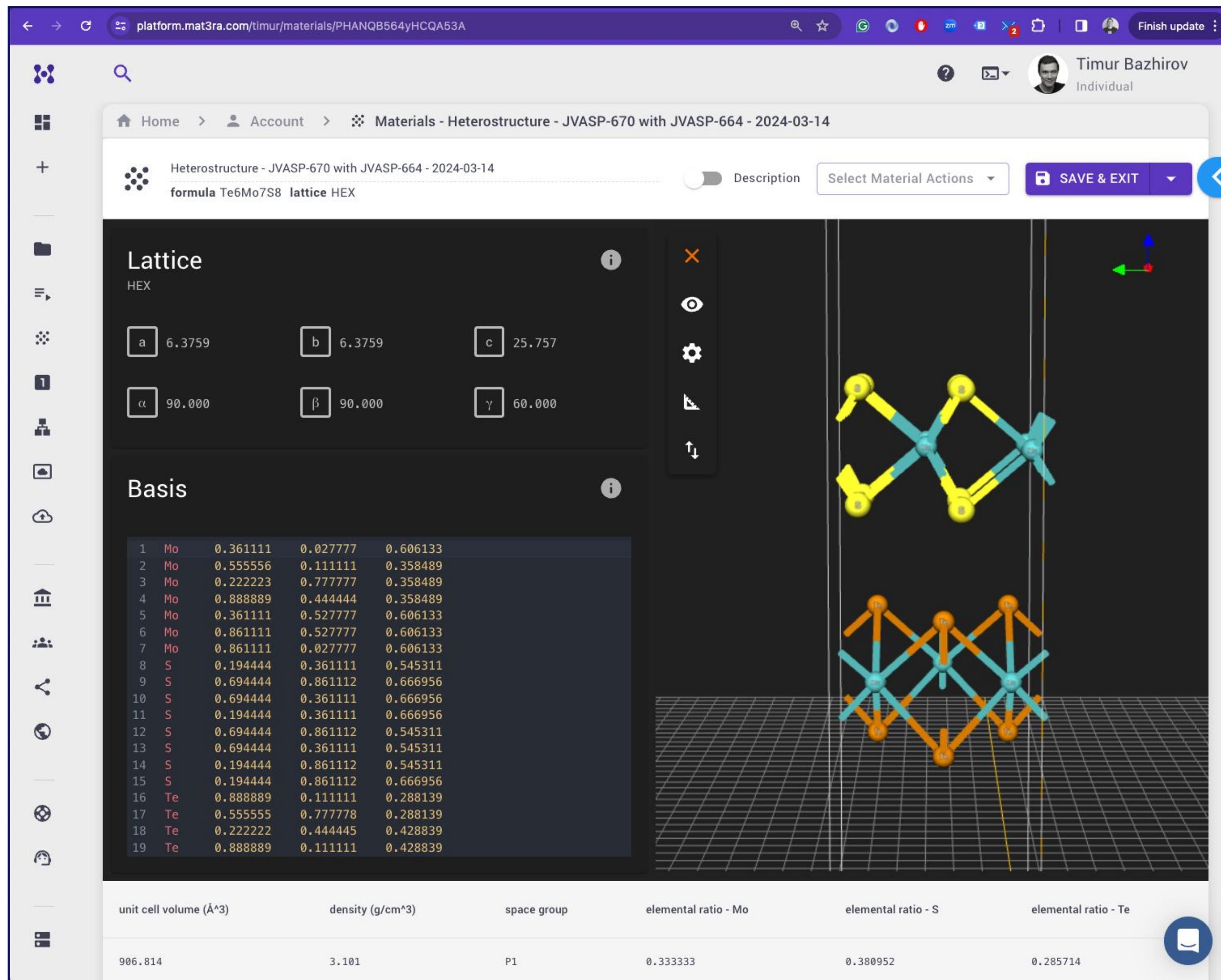
2. Nano-materials - (Proof-of-Concept)

- 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

VALENCE BAND OFFSETS



platform.mat3ra.com/bank/workflows/kXJ9j9piJTddX9FHz

MAT3RA PRO WORKFLOW

Valence Band Offset (2D)
applications: espresso, python

Select Workflow Actions **SAVE**

BS + Avg ESP (Interface)
Type: subworkflow

Flowchart ID: d10ae4e497772ad3cf4a8e25

OVERVIEW **UNITS**

CLONE **DELETE**

Find ESP Values (Interface)
Type: subworkflow

Flowchart ID: ed93beb546e8c2447847ba5

OVERVIEW **UNITS**

CLONE **DELETE**

BS + Avg ESP (interface left)
Type: subworkflow

Flowchart ID: d65de2af2431353b3d0f7b93

OVERVIEW **UNITS**

CLONE **DELETE**

Find ESP Value (Interface left)
Type: subworkflow

Flowchart ID: 2db6a6dc007736d99112fe9c

OVERVIEW **UNITS**

CLONE **DELETE**

BS + Avg ESP (interface right)
Type: subworkflow

Flowchart ID: 7e39825766b0686a04c525de

OVERVIEW **UNITS**

CLONE **DELETE**

BS + Avg ESP (Interface)
espresso

OVERVIEW **IMPORTANT SETTINGS** **DETAILED VIEW** **COMPUTE**

DETAILS

UNITS Select Unit Actions

01 Set Material Index (Inte... Idle
Type: assignment

Flowchart ID: 17dad238dfdcbb95f6aba7c3

EDIT **CLONE** **DELETE**

02 pw_scf Idle
Type: execution

Flowchart ID: bac1466b-a864-468d-915c-e76a5fed5...

EDIT **CLONE** **DELETE**

03 pw_bands Idle
Type: execution

Flowchart ID: pw-bands-calculate-band-gap

EDIT **CLONE** **DELETE**

04 Select indirect band gap Idle
Type: assignment

Flowchart ID: 409bd1a1c2bf584123fec906e

EDIT **CLONE** **DELETE**

05 Set Valence Band Maxi... Idle
Type: assignment

Flowchart ID: 9ad7573ac3c8ae91cb1fa297

EDIT **CLONE** **DELETE**

06 bands Idle
Type: execution

Flowchart ID: aec69bcd-ed82-4fdc-bb95-45db63e19...

EDIT **CLONE** **DELETE**

07 Electrostatic Potential (... Idle
Type: execution

Flowchart ID: 43d85ba8-cdc7-4436-be8e-39cf93388...

EDIT **CLONE** **DELETE**

08 average ESP Idle
Type: execution

Flowchart ID: average-electrostatic-potential

EDIT **CLONE** **DELETE**

09 Set Macroscopically Av... Idle
Type: assignment

Flowchart ID: 41e5f79c6d061570f69b97a2

EDIT **CLONE** **DELETE**

...



New Job Nov 14, 2022, 18:49 PM

project Default

Select Job Actions

▼

SAVE

1. MATERIALS



Silicon FCC

formula Si lattice FCC

2. WORKFLOW

◀ 1 of 1 ▶

Select Material Actions

▼

3. COMPUTE

Lattice

FCC

a 3.8670

b 3.8670

c 3.8670

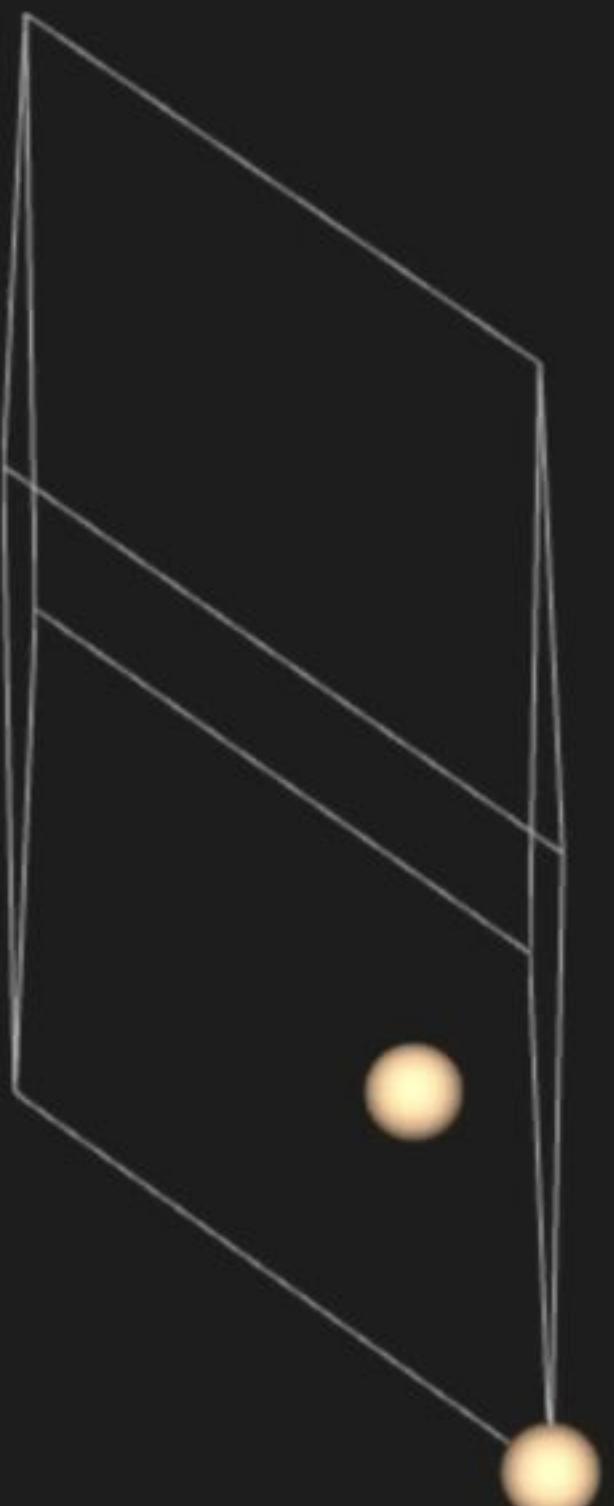
α 60.000

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 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><div>BS + AVG ESP (INTERFACE)</div><div>FIND ESP VALUES (INTERFACE)</div><div>BS + AVG ESP (INTERFACE LEFT)</div><div>FIND ESP VALUE (INTERFACE LEFT)</div><div>BS + AVG ESP (INTERFACE RIGHT)</div><div>FIND ESP VALUE (INTERFACE RIGHT)</div><div>CALCULATE VBO</div></div> | | | | | | | |
|--|--|--|--|--|--|--|--|--|

1-20 of 42 workflows ▲ 0 selected



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 ×



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

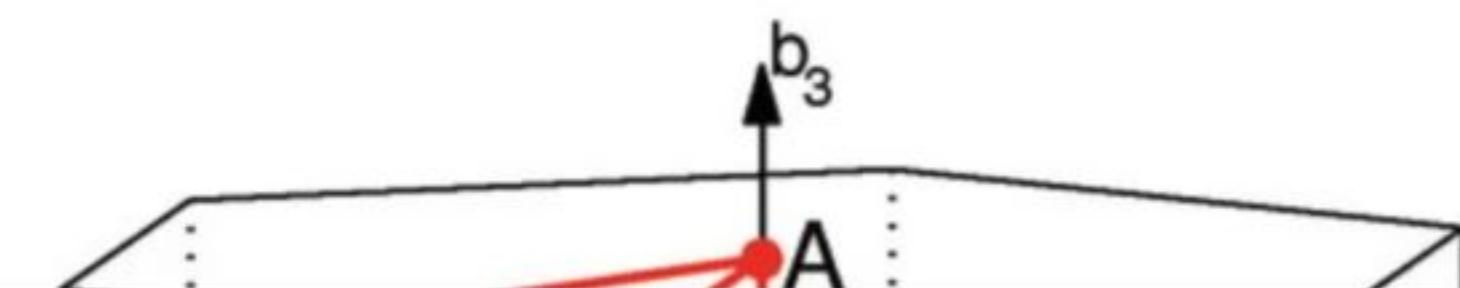
144

 preferKPPRA

Unit 2: pw_bands

kpath

Brillouin zone: HEX





New Job Nov 14, 2022, 18:49 PM

project Default

Select Job Actions



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)



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 | F | Nov 14, 2022 6:52 pm | | | | |

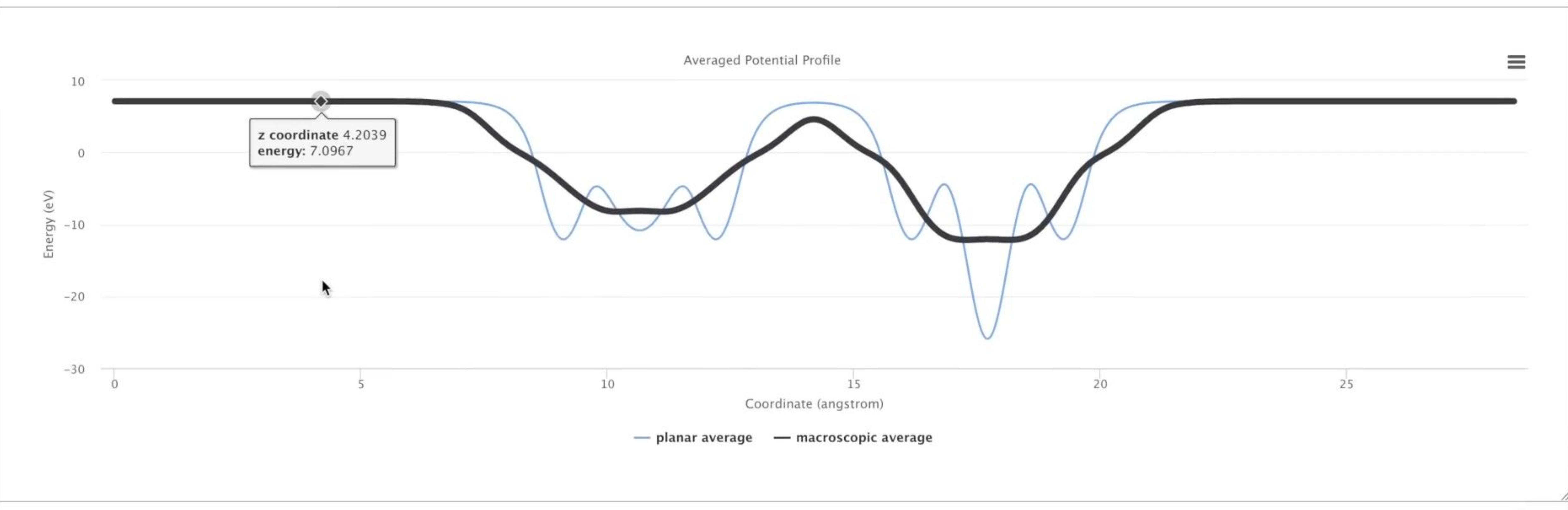
 1-1 of 1 job 0 selected



BS + Avg ESP (Interface) - average ESP

espresso

-



BS + Avg ESP (interface left) - pw_scf

espresso

-



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 >

REST-API USAGE EXAMPLE

Files

dev

Go to file t

- > .github
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 - run_job_using_material_fro...
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 - > materials_designer
 - > materialsproject
 - > python_transformations
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 - > utils
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 - .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())
```

OPEN IN BROWSER

Summary

Join us in building community-driven digital materials R&D ecosystem together

- Mat3ra.com is a **digital ecosystem** accelerating materials R&D by making digital techniques developed by the scientific community accessible & collaborative.
- Our focus is on **modeling and simulations** at the nanoscale (Density Functional Theory, Molecular Dynamics, etc.) coupled with the related AI/ML techniques.
- Mat3ra.com has (1) over 10,000 users, and (2) dozens of customers, including AFRL, Merck KGaA, and Shell. This provided a set of learnings resulting in an **open-source data standards** framework aimed to facilitate FAIR AI-driven R&D.
- Join our informal “Social Hour” **4.45-6p** to learn more and explore collaborative opportunities



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