




Chemiscope 1.0: interactive exploration of atomistic data from analysis to dissemination

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Summary

Chemiscope is an interactive visualization tool for exploring structure-property relationships in molecular and materials datasets (Fraux et al., 2020). It links a map view, e.g. a low-dimensional embedding or property-property scatter plot, to an interactive 3D structure viewer, which streamlines inspection of clusters and outliers by moving between points in feature and property space and the corresponding atomic configurations.

Chemiscope 1.0 turns the original browser-based visualizer into a versatile, multi-purpose tool that fits into Python-centric workflows. The same visualization can be rendered as a standalone web viewer, embedded as a Jupyter widget (Granger & Pérez, 2021; Pérez & Granger, 2007), included in Streamlit web applications, or integrated into Sphinx-built documentation and sphinx-gallery examples for reproducible software manuals (Nájera et al., 2023). Chemiscope 1.0 also provides support for visualizing datasets directly from widely used atomistic Python toolkits, including ASE (Larsen et al., 2017), MDAnalysis (Gowers et al., 2016), stk (Turcuni et al., 2021), and Chemfiles (Fraux et al., 2023).

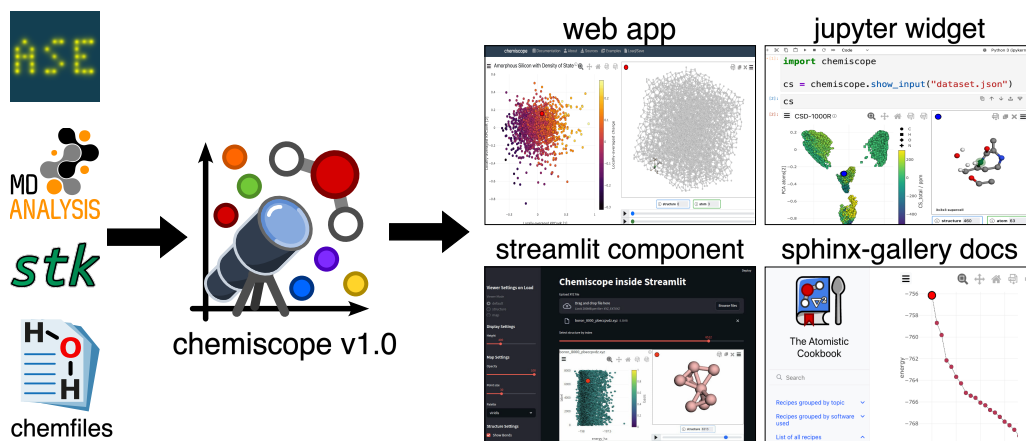


Figure 1: Overview of Chemiscope 1.0 multi-environment support. The Python API accepts structures from ASE, MDAnalysis, stk, and Chemfiles, along with user-defined properties and visualization settings. These inputs can be rendered as an interactive Jupyter widget, embedded in Streamlit applications, integrated into Sphinx documentation, or exported for the standalone web application at chemiscope.org.

Statement of need

Atomistic modeling workflows produce collections of molecular and materials structures together with associated quantities, including energies, forces, charges, and other scalar or tensorial properties. These datasets are commonly explored using post-processing analysis, including property-property correlations (Huang et al., 2020; Würger et al., 2021) and low-dimensional projections (Helfrecht et al., 2020; Hernández-León & Caro, 2024; Jorgensen et al., 2026; Orlov et al., 2025; Tamura et al., 2022), to relate abstract representations to the underlying atomic configurations (Chapman et al., 2022; Nicholas et al., 2020). Interactive visualization provides a practical means to interpret structure-property relationships (Würger et al., 2021), verify computational results, identify unexpected patterns (Xie & Grossman, 2018), and explore learned representations (Cheng et al., 2020; De et al., 2016; Park et al., 2025).

State of the field

Chemiscope has been adopted across multiple atomistic modeling and coarse-grained studies, with interactive viewers shared alongside publications and archived datasets on platforms such as Materials Cloud (Talirz et al., 2020). While complementary visualization tools exist, from desktop applications such as VMD and OVITO (Humphrey et al., 1996; Stukowski, 2010) to WebGL-based molecular viewers such as 3Dmol.js and NGLview (Nguyen et al., 2017; Rego & Koes, 2015), Chemiscope distinguishes itself by providing a single dataset representation and rendering stack that can be reused across multiple contexts. This is especially important in Python-based workflows, where the same visualization is often needed in a Jupyter notebook for analysis, a web view for sharing, and documentation for reproducibility and teaching (Du et al., 2024; Goscinski et al., 2025; Kluyver et al., 2016).

Software design

Chemiscope 1.0 is implemented as a TypeScript visualization library with the Python package providing platform-specific integrations. The Python API can be used to build a Chemiscope dataset from atomic structures, associated properties, and visualization settings, and export it in the JSON schema consumed by the JavaScript renderer. The interface is organized into linked map, structure, and information panels. The map panel uses Plotly.js to render 2D and 3D scatter plots (Plotly Technologies Inc., 2015), the structure panel uses 3Dmol.js for molecular rendering.

The map rendering is a primary performance bottleneck for large datasets. Chemiscope 1.0 introduces adaptive Level of Detail (LOD) rendering for scatter views, which downsample large datasets based on screen-space density, i.e., how many points would overlap in the current view. As users zoom or change view parameters, the displayed subset is updated to preserve both responsiveness and visual structure. In practice, this handles maps with more than 500,000 points on commodity hardware, without requiring users to pre-filter or manually decimate their data. Structure data can also be off-loaded to external files, reducing memory footprint and initial loading time.

Chemiscope 1.0 introduces the possibility of rendering atom-centered shapes to represent vectorial and tensorial properties, including arrows (e.g. dipoles or forces), ellipsoids (e.g. polarizabilities), and user-defined triangular meshes. For biomolecular systems, it supports cartoon representations based on residue and chain information. The structure viewer handles a grid layout for side-by-side comparison of multiple structures or local environments.

In Jupyter notebooks, the viewer is exposed as a widget with bidirectional communication between Python and the JavaScript runtime, implemented via traitlets (Granger & Pérez, 2021; Pérez & Granger, 2007). The widget supports programmatic control of the visualization, including selection synchronization, settings modification, and export of map snapshots.

Users can create a visualization by preparing structures and associated properties and calling `chemiscope.show`:

```
import ase.io
import chemiscope

structures = ase.io.read("trajectory.xyz", ":")

# Extract properties present in the trajectory (e.g. energy, forces)
properties = chemiscope.extract_properties(structures)

# Set default settings for multi-frame trajectories
settings = chemiscope.quick_settings(trajectory=True)

# Display the viewer
chemiscope.show(structures=structures, properties=properties, settings=settings)
```

For web applications built with Streamlit, the Chemiscope component renders a viewer from an in-memory dataset and propagates user interactions (e.g. selection and settings changes) back to Python, coupling to other Streamlit widgets. For reproducible documentation, Chemiscope includes a Sphinx extension that embeds interactive viewers alongside narrative text and executable examples (Nájera et al., 2023).

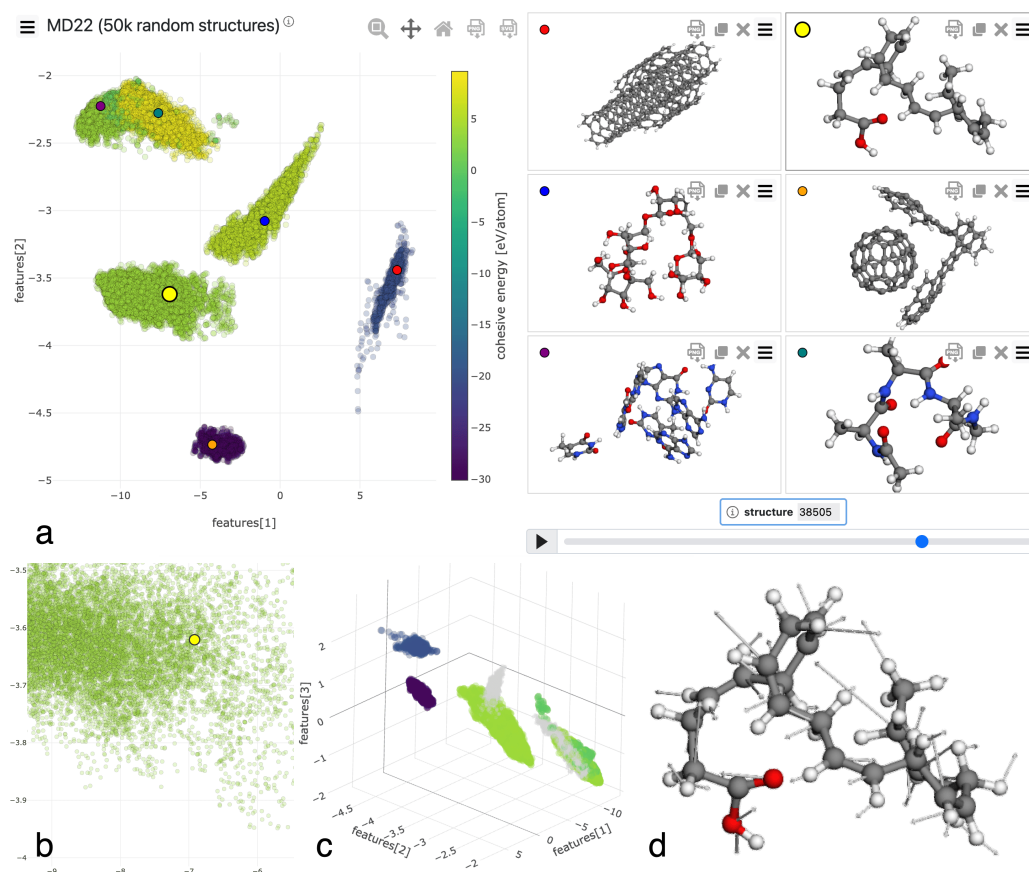


Figure 2: 50k random structures from the MD22 dataset (Chmiela et al., 2023) visualized with Chemiscope by projecting them into the PET-MAD reduced latent space using `chemiscope.explore`. Panel a) shows the Chemiscope widget overall, panel b) a zoom-in of the map demonstrating adaptive level-of-detail rendering, panel c) the 3D view with selective coloring by cohesive energy, and panel d) the shape functionality displaying forces as arrows.

Finally, the package includes an `explore` function that generates interactive visualizations starting from structures alone. It integrates metatomic models (Bigi et al., 2026), particularly the PET-MAD model (Mazitov, Bigi, et al., 2025), which is used by default, to derive informative representations and produce map coordinates without requiring manual descriptor engineering or an explicit dimensionality reduction step (Mazitov, Chorna, et al., 2025):

```
chemiscope.explore(structures, featurizer="pet-mad-1.0")
```

Chemiscope is distributed as an open-source package that can be installed from PyPI, and the default standalone viewer is available online at <https://chemiscope.org> for quick inspection of datasets without local installation. Optional features can be installed via extras: `pip install 'chemiscope[streamlit]'` and `pip install 'chemiscope[explore]'`.

Research impact statement

Chemiscope has been adopted by the atomistic modeling community as a tool for interactive exploration of structure-property relationships. Interactive visualizations built with Chemiscope accompany publications and archived datasets on Materials Cloud (Talirz et al., 2020) and provide citable links that readers can use to explore data beyond static images. As of May 2026, the Materials Cloud Archive lists 19 publications using Chemiscope as an external app (Materials Cloud Archive, 2026).

The tool has been cited in studies spanning machine-learned interatomic potentials and datasets (Batatia et al., 2025; Cheng et al., 2020; He et al., 2025; Keith et al., 2021; Mazitov, Chorna, et al., 2025), coarse-grained molecular representations (Helfrecht et al., 2020; Nicholas et al., 2020), and high-throughput screening of materials (Blaskovits et al., 2024; Gallarati et al., 2022; Jorgensen et al., 2026). Chemiscope is integrated with the metatensor ecosystem (Bigi et al., 2026) through the `chemiscope.explore` function, which uses foundation models like PET-MAD (Mazitov, Bigi, et al., 2025) to generate map coordinates without manual descriptor engineering.

Beyond research papers, Chemiscope serves educational and reproducibility purposes: tutorials and course materials use live widgets to demonstrate dimensionality reduction and structure-property correlations (Goscinski et al., 2025), and Chemiscope viewers can be embedded directly into manuals, as is done in the Atomistic Cookbook recipes (The Atomistic Cookbook, 2026). The Python package reached 5,726 downloads in the last month on PyPI Stats, accessed May 2026 (PyPI Stats for Chemiscope, 2026).

AI usage disclosure

Generative AI tools were used occasionally during software development (e.g. to obtain code suggestions). All AI-generated suggestions were reviewed, modified, and verified by the authors before inclusion, and the authors take full responsibility for the final content of the software.

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