

Resource Summary Report

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Pymatgen

RRID:SCR_016565

Type: Tool

Proper Citation

Pymatgen (RRID:SCR_016565)

Resource Information

URL: <http://www.pymatgen.org/>

Proper Citation: Pymatgen (RRID:SCR_016565)

Description: Python library for materials analysis codes. Defines core object representations for structures and molecules.

Abbreviations: Pymatgen

Synonyms: PYthon MATerials GENomics

Resource Type: software toolkit, software resource, software library

Defining Citation: [DOI:10.1016/j.commatsci.2012.10.028](https://doi.org/10.1016/j.commatsci.2012.10.028)

Keywords: material, analysis, code, core, object, representation, structure, molecule

Availability: Free, Available for download, Freely available.

Resource Name: Pymatgen

Resource ID: SCR_016565

Alternate URLs: <https://github.com/materialsproject/pymatgen>

License: MIT License

Record Creation Time: 20220129T080331+0000

Record Last Update: 20260819T044442+0000

Ratings and Alerts

No rating or validation information has been found for Pymatgen.

No alerts have been found for Pymatgen.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 26 mentions in open access literature.

Listed below are recent publications. The full list is available at [dkNET](#) .

Park J, et al. (2026) Improved Air Stability of Li Argyrodites Through PS4 3- Rotation Suppression by Al and Se Co-Substitution for All-Solid-State Batteries. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 13(11), e19093.

Shermukhamedov S, et al. (2026) Machine-Learning Ice Spectra: From 1 to 256 Features. Journal of chemical theory and computation, 22(4), 1834.

Guan C, et al. (2026) Triggering dynamically disordered lithium sublattice in superionic conductors. Nature communications, 17(1).

Song Z, et al. (2025) Inverse design of promising electrocatalysts for CO2 reduction via generative models and bird swarm algorithm. Nature communications, 16(1), 1053.

Wang H, et al. (2025) Machine learning and DFT database for C-H dissociation on single-atom alloy surfaces in methane decomposition. Scientific data, 12(1), 648.

Miao L, et al. (2025) W/Mo/Cr Doping Modulates the Negative-Positive Inversion Gas Sensing Behavior of VO₂(M1). ACS sensors, 10(1), 526.

Choudhary S, et al. (2025) Ion coordination and migration mechanisms in alkali metal complex borohydride-based solid electrolytes. Communications chemistry, 8(1), 123.

Banerjee S, et al. (2025) Non-local interactions determine local structure and lithium diffusion in solid electrolytes. Nature communications, 16(1), 1672.

Liu X, et al. (2025) 3D Porous Zinc Scaffold Anodes for Enhanced Stability and Performance in Zinc-Ion Energy Storage Systems. ACS nano, 19(28), 26147.

Zhang T, et al. (2025) SuperBand: an Electronic-band and Fermi surface structure database of superconductors. Scientific data, 12(1), 744.

Truong E, et al. (2025) Accelerating ion transport in polycrystalline conductors: On pores and grain boundaries. Science advances, 11(20), eadt7795.

Sommer T, et al. (2025) Beyond chemical structures: lessons and guiding principles for the next generation of molecular databases. Chemical science, 16(3), 1002.

Luo X, et al. (2025) CrystalFlow: a flow-based generative model for crystalline materials. Nature communications, 16(1), 9267.

Won J, et al. (2025) Mapping cation-eutaxy ternary with a phenomenological model. Nature communications, 16(1), 5634.

Steinberg Y, et al. (2024) Composition and Structure of the solid electrolyte interphase on Na-Ion Anodes Revealed by Exo- and Endogenous Dynamic Nuclear Polarization???NMR Spectroscopy. Journal of the American Chemical Society, 146(35), 24476.

Zhong J, et al. (2024) Coordination engineering for iron-based hexacyanoferrate as a high-stability cathode for sodium-ion batteries. Proceedings of the National Academy of Sciences of the United States of America, 121(31), e2319193121.

Chen Y, et al. (2024) Ion Transport at Polymer-Argyrodite Interfaces. ACS applied materials & interfaces, 16(36), 48223.

Omidvar M, et al. (2024) Accelerated discovery of perovskite solid solutions through automated materials synthesis and characterization. Nature communications, 15(1), 6554.

Guo H, et al. (2023) Simulated sulfur K-edge X-ray absorption spectroscopy database of lithium thiophosphate solid electrolytes. Scientific data, 10(1), 349.

Wu Y, et al. (2022) Data-driven discovery of high performance layered van der Waals piezoelectric NbOI₂. Nature communications, 13(1), 1884.