Resource Summary Report

Generated by RRID on Aug 6, 2026

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 library, software resource

Defining Citation: DOI: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: 20260806T054641+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 23 mentions in open access literature.

Listed below are recent publications. The full list is available at RRID .

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.

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.

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.

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

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.

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

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

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

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

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

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

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.

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.

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

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

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.

Wang Y, et al. (2022) Integrated High-Throughput and Machine Learning Methods to Accelerate Discovery of Molten Salt Corrosion-Resistant Alloys. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 9(20), e2200370.

Zhou Z, et al. (2022) Tuning the Electronic, Ion Transport, and Stability Properties of Li-rich Manganese-based Oxide Materials with Oxide Perovskite Coatings: A First-Principles Computational Study. ACS applied materials & interfaces, 14(32), 37009.

Wu EA, et al. (2021) A stable cathode-solid electrolyte composite for high-voltage, long-cycle-life solid-state sodium-ion batteries. Nature communications, 12(1), 1256.