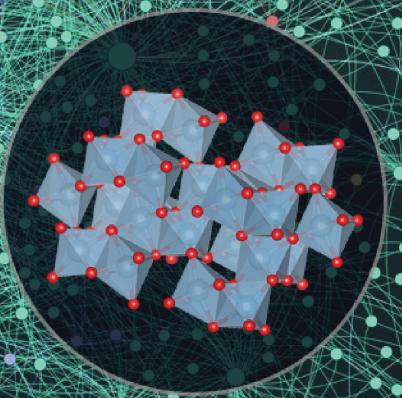
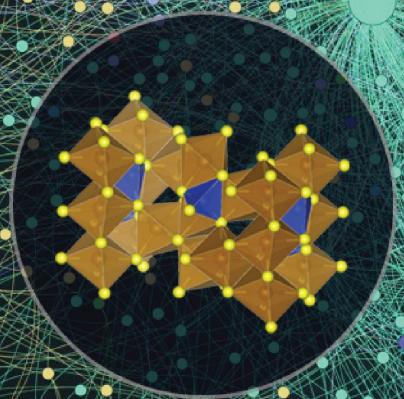
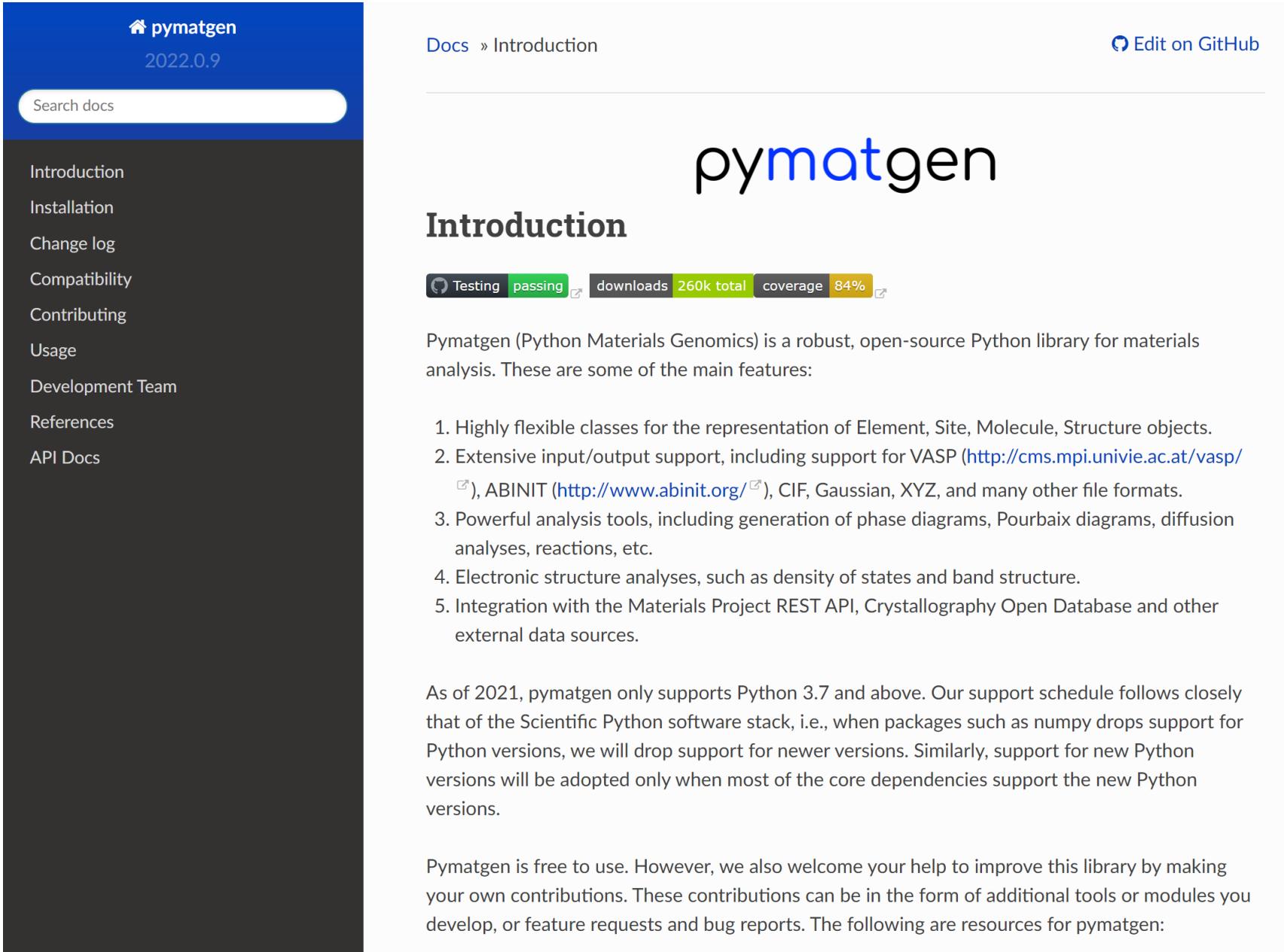


Materials Data: Access



We will use the pymatgen library



The screenshot shows the official pymatgen documentation website. At the top left is the logo "pymatgen" with a house icon, followed by the text "2022.0.9". A search bar labeled "Search docs" is positioned below the logo. On the right side of the header are links for "Docs" (highlighted in blue) and "Edit on GitHub". The main content area features a large title "pymatgen" with "pymat" in blue and "gen" in black. Below it is a section titled "Introduction". Underneath the title are several status indicators: "Testing passing" (green button), "downloads 260k total" (black button), and "coverage 84%" (yellow button). The main text explains what Pymatgen is: "Pymatgen (Python Materials Genomics) is a robust, open-source Python library for materials analysis. These are some of the main features:". A numbered list follows, detailing the library's capabilities: 1. Highly flexible classes for the representation of Element, Site, Molecule, Structure objects. 2. Extensive input/output support, including support for VASP (<http://cms.mpi.univie.ac.at/vasp/>), ABINIT (<http://www.abinit.org/>), CIF, Gaussian, XYZ, and many other file formats. 3. Powerful analysis tools, including generation of phase diagrams, Pourbaix diagrams, diffusion analyses, reactions, etc. 4. Electronic structure analyses, such as density of states and band structure. 5. Integration with the Materials Project REST API, Crystallography Open Database and other external data sources. A note at the bottom states: "As of 2021, pymatgen only supports Python 3.7 and above. Our support schedule follows closely that of the Scientific Python software stack, i.e., when packages such as numpy drops support for Python versions, we will drop support for newer versions. Similarly, support for new Python versions will be adopted only when most of the core dependencies support the new Python versions." Finally, a call to action at the bottom encourages users to contribute: "Pymatgen is free to use. However, we also welcome your help to improve this library by making your own contributions. These contributions can be in the form of additional tools or modules you develop, or feature requests and bug reports. The following are resources for pymatgen:".

Machine Learning: Tasks and Types

