sumo: Command-line plotting tools for ab initio calculations

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Ab initio electronic structure modelling is capable of providing an insight into the fundamental properties of materials, at a resultion beyond that of experimental techinques. The optoelectronic properties of a compound can be described through several key descriptions, including: density of states diagrams, which provide information on the orbital character of frontier bonding; band structures, which afford an indication of carrier transport properties; and optical absorption spectra, which can be used to assess the wavelengths of light a material will transmit or absorb. An understanding of these fundamental properties is crucial when selecting or optimising materials for particular applications, including photovoltaics, transparent conductors, and thermoelectrics.

Most common ab initio calculation software, such as Vienna ab initio Simulation Package (VASP) and Quantum Espresso, write raw data which require post-processing steps to plot or convert into a human-readable format. Several packages exist that facilitate the creation and plotting of such diagrams. Python libraries, such as Python Materials Genomics (pymatgen) and Atomic Simulation Environment (ase), provide powerful interfaces for plotting and data analysis but require the user to be profficient in Python to use effectively. Conversely, programs which provide a graphical user interface, such as p4vasp and XCrySDen, are easy to use but are not conducive to working on the command line.

`sumo`

`sumo` is a set of command line scripts and a corresponding Python API, for publication-ready plotting and analysis of ab initio calculation data.

- publication ready diagrams
- customisable
- quick and easy to use
- python api available
- list of commands available
- example of band structure, dos and optics plots