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sumo: Command-line tools for plotting and analysis of *ab initio* calculations

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Software

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Ab initio electronic structure modelling is capable of providing an insight into the fundamental properties of materials, at a resolution beyond that of experimental techniques. The optoelectronic properties of a compound are analysed through several key descriptions, including: density-of-states distributions, which provide information on the orbital character of bonding; band structure diagrams, which indicate carrier transport properties; and optical absorption spectra, which are 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 (Ganose, Savory, and Scanlon 2017), transparent conductors (Ganose and Scanlon 2016), and thermoelectrics (Gorai, Stevanović, and Toberer 2017).

Most common *ab initio* calculation software, such as Vienna *ab initio* Simulation Package (VASP) (Kresse and Furthmüller 1996) and Quantum Espresso (Giannozzi et al. 2009), write raw data which require post-processing 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) (Ong et al. 2013) and Atomic Simulation Environment (ase) (Larsen et al. 2017), provide powerful interfaces for plotting and data analysis but require the user to be proficient in Python to use effectively. Conversely, programs which provide a graphical user interface, such as p4vasp (Dubay 2018) and XCrySDen (Kokalj 1999), are easy to use but are not conducive to working on the command line. The purpose of this package is to provide an intermediate solution that is trivial to use but still provides the flexibility needed for a broad range of analysis modes.

`sumo`

`sumo` is a set of command-line tools for publication-ready plotting and analysis of *ab initio* calculation data. The code includes a fully-documented Python module, upon which the command-line scripts are built. `sumo` currently only supports VASP, however, extending the code to other *ab initio* calculators is planned for future releases. The code relies on several open-source Python packages for common tasks, including pymatgen for data loading (Ong et al. 2013), spglib for symmetry analysis (Togo 2013), and matplotlib for plotting (Hunter 2007).

The main plotting functionality of `sumo` includes density of states plots, electronic and phonon band structure diagrams, and optical absorption spectra (Figure 1). The code has been designed to allow for significant customisation of plots, including the ability to produce projected density of states and orbital resolved band structures. The code additionally supplies a tool for generating k-point paths along high-symmetry directions in

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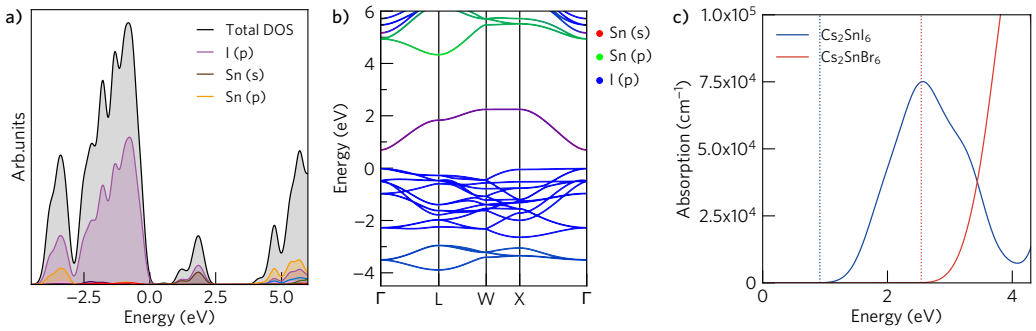

Figure 1: Diagrams produced by `sumo`. a) Density of states, b) projected band structure, and c) optical absorption spectra.

the Brillouin zone, with the ability to write the necessary input files required to perform the calculations in VASP. Crucially, this tool allows a single band structure plot to be split into several *ab initio* calculations, as is essential when dealing with large materials or restrictive batch systems. Lastly, a script is provided to extract information from semiconductor band structures, including direct and indirect band gaps, band edge locations, and parabolic and non-parabolic effective masses.

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