sumo: Command-line tools for plotting and analysis of 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 resolution beyond that of experimental techniques. 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 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 (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 1996) and Quantum Espresso (Giannozzi et al. 2009), 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) (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 aim of this work 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 the VASP program, however, extending the code to other ab initio calculators

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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 functions (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 the Brillouin zone, with the ability to write the necessary input files required to perform the calculations in VASP. Crucially, this tool supports splitting up band structures into several parts, as is essential when dealing with ambitious calculations 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.
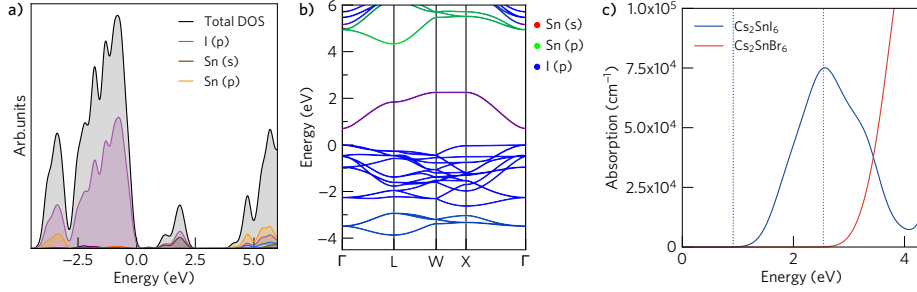

Figure 1: Diagrams produced by `sumo`. a) Density of states, b) projected band structure, and c) optical absorption spectra.

Acknowledgements

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