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

Alex M Ganose[1, 2, 3], **Adam J Jackson**[1], **and David O Scanlon**[1, 2, 3]

1 Dept of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, UK **2** Diamond Light Source Ltd., Diamond House, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, UK **3** Thomas Young Centre, University College London, Gower Street, London WC1E 6BT, UK

DOI: 10.21105/joss.00717

Software

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Submitted: 17 April 2018
Published: 07 August 2018

Ab initio electronic structure modelling is capable of providing an insight into the fundamental properties of solid-state 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, & Scanlon, 2017), transparent conductors (Ganose & Scanlon, 2016), and thermoelectrics (Gorai, Stevanović, & Toberer, 2017).

Most common *ab initio* calculation software for analysing crystalline materials with periodic boundary condictions, such as Vienna *ab initio* Simulation Package (VASP) (Kresse & 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 for solid-state materials. 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 solid-state *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 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

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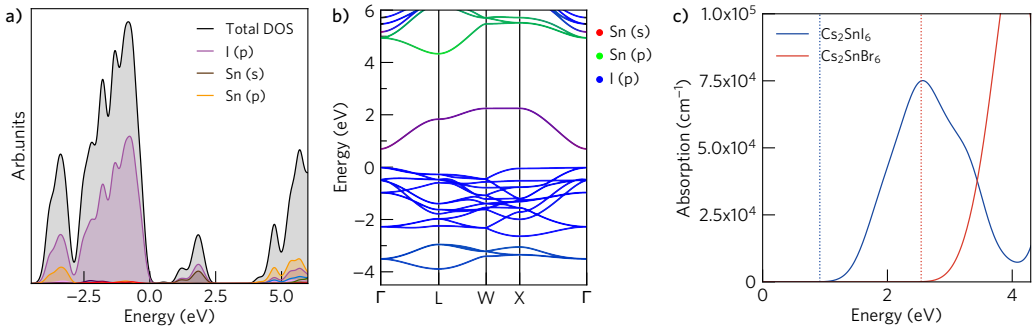

Figure 1: Diagrams produced by `sumo`. a) Density of states, b) projected band structure, and c) optical absorption spectra.

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.

Acknowledgements

DOS acknowledges support from the EPSRC (EP/N01572X/1). DOS acknowledges support from the European Research Council, ERC (grant no. 758345). DOS acknowledges membership of the Materials Design Network. AMG acknowledges Diamond Light Source for the co-sponsorship of a studentship on the EPSRC Centre for Doctoral Training in Molecular Modelling and Materials Science (EP/L015862/1).

We acknowledge useful discussions with Zhenyu Wang, Benjamin Morgan, and Jonathan Skelton. Feature requests and user testing came from Benjamin Williamson, Christopher Savory and James Pegg.

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