bsym: A basic symmetry module

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A large number of problems in materials science concern the configurational disorder of atoms. Examples include describing mixing of alloys (Ganose and Scanlon 2016); identifying prefferred arrangements in crystals of non-dilute point defects, dopants, or intercalated atoms (Morgan and Watson 2011, Grieshammer et al. (2014), Dalton, Belak, and Van Der Ven (2012)); or predicting crystal surface structures or the arrangements of adsorbed atoms (Morgan, Carrasco, and Teobaldi 2016).

Computational modelling can provide useful insight into problems such as these. For a given atomic geometry, relative energies, or other such properties, can be directly calculated. Repeating these calculations across a range of possible structures can be used to identify which atom arrangements are more or less likely, or be used to construct a statistical description giving an ensemble average. For bulk materials with approximately random disorder (ideal mixing) special quasi-random structures can be used to model the effects of disorder in a single periodic system (Zunger et al. 1990). Where disorder is not random, however, contributions from different atomic configurations need to be explicitly considered. One approach is to model the system energy via an effective Hamiltonian (for example, parameterised using cluster expansion methods), and then to perform Monte Carlo simulations (Lerch et al. 2009, Walle and Ceder (2002), ("CASM, V0.2.1" 2017), Ludwig et al. (2011)). This approach depends on the accuracy of the effective Hamiltonian, and is particularly suited to systems where short-range interactions dominate the total energy. An alternative is to explicitly consider all possible configurations of relevant atoms within a reduced configurational space (e.g. a computationally tractable supercell) (Grau-Crespo et al. 2007, Tompsett and Islam (2013)).

In this approach, the overall computational cost can be greatly reduced by considering only *symmetry inequivalent* configurations. If, for each of these unique structures, the number of symmetry-equivalent configurations is known, then in addition to individual enthalpies, configurational entropies, and hence free energies, may be calculated (Grau-Crespo et al. 2007).

`bsym`

`bsym` (Morgan 2016) is a Python module for performing symmetry-based manipulations on arbitrary configuration vector spaces. The code includes an efficient implementation of the algorithm described by Grau-Crespo *et al.*, for enumerating symmetry inequivalent configurations (Grau-Crespo et al. 2007). For treating the specific case of site-disorder in crystals, `bsym` includes an interface for working with `pymatgen Structure` objects (Ong et al. 2013), which allows simple construction of sets of symmetry operations for crystal structures, and conversion to and from a range of standard file formats for recording crystal structures and for inputs for a range of atomistic modelling codes. The core classes describe objects corresponding to an abstracted matrix representation of configurational vector spaces and their symmetry properties. This means `bsym` can be readily used for analysis in other classes of problems, including molecular point groups, crystal surface symmetries (2D space groups), and graph theoretical colouring problems.

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