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LobsterPy: A package to automatically analyze LOBSTER runs

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Software

- Review
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Summary

The LOBSTER software aids in extracting quantum-chemical bonding information from materials by projecting the plane-wave based wave functions from density functional theory (DFT) onto an atomic orbital basis. LobsterEnv, a module implemented in pymatgen(Ong et al., 2013) by some of the authors of this package, facilitates the use of quantum-chemical bonding information obtained from LOBSTER calculations to identify neighbors and coordination environments. *LobsterPy* is a Python package that offers a set of convenient tools to further analyze and summarize the LobsterEnv outputs in the form of JSONs that are easy to interpret and process. These tools enable the estimation of (anti) bonding contributions, generation of textual descriptions, and visualization of LOBSTER computation results. Since its first release, both *LobsterPy* and *LobsterEnv* capabilities have been extended significantly. Unlike earlier versions, which could only automatically analyze Crystal Orbital Hamilton Populations (COHPs)(Dronskowski & Blöchl, 1993), both can now also analyze Crystal Orbital Overlap Populations (COOP)(Hughbanks & Hoffmann, 1983) and Crystal Orbital Bond Index (COBI)(Müller et al., 2021). Extracting the information about the most important orbitals contributing to the bonds is optional, and users can enable it as needed. Additionally, bonding-based features for machine-learning (ML) studies can be engineered via the sub-packages "featurize" and "structuregraphs". Alongside its Python interface, it also provides an easy-to-use command line interface (CLI) that runs automatic analysis of the computations and generates a summary of results and publication-ready figures.

LobsterPy has been used to produce the results in (Chen et al., 2024; Naik et al., 2023; Ngo et al., 2023) and is also part of (*Atomate2*, 2023) bonding analysis workflow for generating bonding analysis data in a format compatible with the Materials Project(Jain et al., 2013) API.

Statement of need

Although the notion of "bonds" might seem unusual from a physicist's point of view, chemists have been employing it routinely to explain various chemical phenomena and materials properties.(Burdett, 1995; Das et al., 2023; Dronskowski, 2023; Ertural et al., 2022; Hoffmann, 1987; Hu et al., 2023) With the recent advances in automation frameworks for high-throughput computational investigations, bonding analysis for thousands of crystalline materials can be performed with few lines of code.(George et al., 2022) This automation helps reduce the common mistakes inexperienced users make while performing bonding analysis. However, it is also essential to systematically generate inputs and post-process the output files consistently to have reliable and reproducible results. Furthermore, transforming the data from these

high-throughput bonding analysis calculations into a format suitable for ML studies should benefit data-driven material science research. *LobsterPy* aims to fulfill this need.

Features

- Generate summarized bonding analysis JSONs and text descriptions based on COHPs (ICOHPs), COBIs (ICOBIs), and COOPs (ICOOPs)
- Generate static and interactive plots of the most relevant COHPs, COBIs, and COOPs
- Customizable plotters for visualization of COHPs (ICOHPs), COBIs (ICOBIs), COOPs (ICOOPs) and DOS
- Benchmark LOBSTER calculation quality and generate corresponding JSONs and text descriptions
- Create inputs for LOBSTER calculations from VASP files
- Extract features from LOBSTER calculation files to be used for ML studies
- Perform automatic bonding analysis and plotting via inherent command line interface app.

Availability

LobsterPy can also be found on PyPI. Detailed software documentation, including installation instructions and implementation details are provided. The package also includes tutorials illustrating all the basic and advanced functionalities.

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