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LobsterPy: A package to automatically analyze LOBSTER runs

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Software

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Summary

The LOBSTER (Deringer et al., 2011; Maintz et al., 2013, 2016; Nelson et al., 2020) 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 Ngo et al. (2023), Chen et al. (2024), Naik et al. (2023), and it 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.

Similar and Related Software

LobsterPy can be seen to be similar in spirit to sumo (Ganose et al., 2018), as both provide Python tools to analyze and visualize data related to the electronic structure that are based on ab initio calculations. Other software packages that enable visualizing results specifically from the LOBSTER software are wxDragon (Eck, 1994–2020) and *Abipy* (2021). LobsterPy differs from these two packages by providing further analysis of the calculations, interpretable text summaries, and featurizers for ML studies besides plotting the data.

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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References

Abipy. (2021). https://github.com/abinit/abipy

Atomate2. (2023). https://github.com/materialsproject/atomate2

Burdett, J. K. (1995). *Chemical bonding in solids*. Oxford University Press.

Chen, B., Li, J., Wang, X., Shi, M., Sun, T., Xia, M., Ding, K., Liu, J., Li, J., Tian, H., & others. (2024). Insights into the heterogeneous nuclei of an ultrafast-crystallizing glassy solid. *Advanced Functional Materials*, 2314565. https://doi.org/10.1002/adfm.202314565

Das, A., Pal, K., Acharyya, P., Das, S., Maji, K., & Biswas, K. (2023). Strong antibonding i (p)–cu (d) states lead to intrinsically low thermal conductivity in CuBiI4. *Journal of the American Chemical Society*, *145*(2), 1349–1358. https://doi.org/10.1021/jacs.2c11908

Deringer, V. L., Tchougréeff, A. L., & Dronskowski, R. (2011). Crystal orbital hamilton population (COHP) analysis as projected from plane-wave basis sets. *The Journal of Physical Chemistry A*, *115*(21), 5461–5466. https://doi.org/10.1021/jp202489s

Dronskowski, R. (2023). *Chemical bonding: From plane waves via atomic orbitals*. Walter de Gruyter GmbH & Co KG. https://doi.org/10.1515/9783111167213

Dronskowski, R., & Blöchl, P. E. (1993). Crystal orbital hamilton populations (COHP): Energy-resolved visualization of chemical bonding in solids based on density-functional calculations. *The Journal of Physical Chemistry*, *97*(33), 8617–8624. https://doi.org/10.1021/j100135a014

Eck, B. (1994–2020). *wxDragon, version 2.2.2*. RWTH Aachen University. https://schmeling.ac.rwth-aachen.de/cohp/index.php?menuID=6

Ertural, C., Stoffel, R. P., Müller, P. C., Vogt, C. A., & Dronskowski, R. (2022). First-principles plane-wave-based exploration of cathode and anode materials for li-and na-ion batteries involving complex nitrogen-based anions. *Chemistry of Materials*, *34*(2), 652–668. https://doi.org/10.1021/acs.chemmater.1c03349

Ganose, A. M., Jackson, A. J., & Scanlon, D. O. (2018). Sumo: Command-line tools for plotting and analysis of periodic *ab initio* calculations. *Journal of Open Source Software*, *3*(28), 717. https://doi.org/10.21105/joss.00717

George, J., Petretto, G., Naik, A., Esters, M., Jackson, A. J., Nelson, R., Dronskowski, R., Rignanese, G.-M., & Hautier, G. (2022). Automated bonding analysis with crystal orbital hamilton populations. *ChemPlusChem*, *87*(11), e202200123. https://doi.org/10.1002/cplu.202200123

Hoffmann, R. (1987). How chemistry and physics meet in the solid state. *Angewandte Chemie International Edition in English*, *26*(9), 846–878. https://doi.org/10.1002/anie.198708461

Hu, C., Zhou, L., Hu, X., Lv, B., & Gao, Z. (2023). Mechanism of the low thermal conductivity in novel two-dimensional NaCuSe. *Applied Surface Science*, *613*, 156064. https://doi.org/10.1016/j.apsusc.2022.156064

Hughbanks, T., & Hoffmann, R. (1983). Chains of trans-edge-sharing molybdenum octahedra: Metal-metal bonding in extended systems. *Journal of the American Chemical Society*, *105*(11), 3528–3537. https://doi.org/10.1021/ja00349a027

Jain, A., Ong, S. P., Hautier, G., Chen, W., Richards, W. D., Dacek, S., Cholia, S., Gunter, D., Skinner, D., Ceder, G., & Persson, K. A. (2013). Commentary: The materials project: A materials genome approach to accelerating materials innovation. *APL Materials*, *1*(1). https://doi.org/10.1063/1.4812323

Maintz, S., Deringer, V. L., Tchougréeff, A. L., & Dronskowski, R. (2013). Analytic projection from plane-wave and PAW wavefunctions and application to chemical-bonding analysis in solids. *Journal of Computational Chemistry*, *34*(29), 2557–2567. https://doi.org/10.1002/jcc.23424

Maintz, S., Deringer, V. L., Tchougréeff, A. L., & Dronskowski, R. (2016). LOBSTER: A tool to extract chemical bonding from plane-wave based DFT. In *Journal of Computational Chemistry* (No. 11; Vol. 37, pp. 1030–1035). Wiley Online Library. https://doi.org/10.1002/jcc.24300

Müller, P. C., Ertural, C., Hempelmann, J., & Dronskowski, R. (2021). Crystal orbital bond index: Covalent bond orders in solids. *The Journal of Physical Chemistry C*, *125*(14), 7959–7970. https://doi.org/10.1021/acs.jpcc.1c00718

Naik, Aakash Ashok, Ertural, Christina, Dhamrait, N., Benner, P., & George, J. (2023). A quantum-chemical bonding database for solid-state materials. *Scientific Data*, *10*(1), 610. https://doi.org/10.1038/s41597-023-02477-5

Nelson, R., Ertural, C., George, J., Deringer, V. L., Hautier, G., & Dronskowski, R. (2020). LOBSTER: Local orbital projections, atomic charges, and chemical-bonding analysis from projector-augmented-wave-based density-functional theory. *Journal of Computational Chemistry*, *41*(21), 1931–1940.

Ngo, H. M., Pal, U., Kang, Y. S., & Ok, K. M. (2023). DFT-based study for the enhancement of CO2 adsorption on metal-doped nitrogen-enriched polytriazines. *ACS Omega*, *8*(9), 8876–8884. https://doi.org/10.1021/acsomega.3c00395

Ong, S. P., Richards, W. D., Jain, A., Hautier, G., Kocher, M., Cholia, S., Gunter, D., Chevrier, V. L., Persson, K. A., & Ceder, G. (2013). Python materials genomics (pymatgen): A robust, open-source python library for materials analysis. *Computational Materials Science*, *68*, 314–319. https://doi.org/10.1016/j.commatsci.2012.10.028