# Application of Abduction in Energy Functional Discovery for Density Functional Theory

**Yu-Cong He**[1], **Wang-Zhou Dai**[1]

[1]The State Key Laboratory of Novel Software Technology
[1]School of Intelligence Science and Technology, Nanjing University

## Abstract

Density Functional Theory (DFT) is the most widely used computational method in materials science for estimating the approximate solution to Schrödinger equation. However, classical DFT methods are usually computationally inefficient. The key to improving DFT is designing effective yet accurate energy-density functionals ($E(\rho)$). The main challenge is the excessively large hypothesis space of potential functions, which is constructed upon large-scale physical background knowledge. We propose an abduction-based method to automatically design better $E(\rho)$ for DFT. Specifically, our method combines a neural network heuristic function and symbolic abduction module to search for the potential function to explain the experimental data. The abduction heuristics can be trained from the closed loop of trials and errors. Finally, it provides theoretical interpretable results.

## Summary

DFT approximates the Schrödinger equation by designing various energy-density functionals, and solve it through self-consistent calculations [3]. Exchange-correlation potential ($E_{xc}(\rho)$) is one of the most important functionals in DFT. However, the currently used $E_{xc}(\rho)$ still results in unavoidable errors (eg. underestimate band gap, which is a basic property of materials) [1]. It's crucial to discover new forms of $E_{xc}(\rho)$ to improve DFT. However, discovering a new functionals is a lengthy and challenging task for humans and current data-driven machine learning methods also struggle to do this effectively.

We propose a $E_{xc}(\rho)$ discovery method based on abductive reasoning, which is inspired by Abductive Meta-Interpretive Learning (MetaAbd) [2]. MetaAbd discovers new interpretation of unknown phenomenon by combining higher-order logic and first-order logic abduction. Figure 1 outlines our method, starts from the Goal Functional. Firstly, the model uses a learnable heuristic module to abduces a hypothesis about the goal functional based on the Knowledge Library. Secondly, the model uses experimental data to estimate the parameters and then validates the hypothesized functional. It will returns to the first step if any step fail.

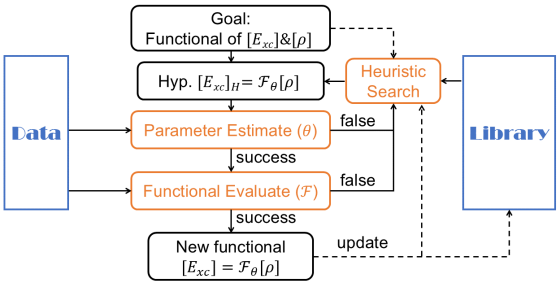


Figure 1: a $E_{xc}(\rho)$ discovery method based on abduction. Yellow section represents the learnable module. Solid lines represent computational process; dashed lines represent information transfer paths.

Finally, if the validation is successful, the newly discovered functional is output and added to the Knowledge Library for use in subsequent processes.

Research in materials science is founded on the explanation of phenomena through human heuristic induction. Our approach aims at extending this capability to computers, and towards to establish a general framework for AI in the field of scientific discovery.

## References

[1] Cohen, A. J.; Mori-Sánchez, P.; and Yang, W. 2012. Challenges for density functional theory. *Chemical reviews*, 112(1): 289–320.

[2] Dai, W.-Z.; and Muggleton, S. 2021. Abductive Knowledge Induction from Raw Data. In *Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence*, 1845–1851. International Joint Conferences on Artificial Intelligence Organization.

[3] He, Y.; and Zhou, J. 2022. First-principles study on the ultralow lattice thermal conductivity of BiSeI. *Physica B: Condensed Matter*, 646: 414278.