

PWDFT.jl: A Julia package for electronic structure calculation using density functional theory and plane wave basis

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**ABSTRACT**

We describe the implementation of PWDFT.jl, a package for electronic structure calculations written using Julia programming language using plane wave basis set and pseudopotentials. In this package, typical Kohn-Sham density functional theory (KSDFT) is divided into three steps: instantiation of an atomistic models, initialization of Kohn-Sham Hamiltonian, and self-consistent field (SCF) calculations. PWDFT.jl is allows user to write their own SCF or alternative methods by providing implementation several basic operations such as wave function orthogonalization, action of kinetic and potential operators to wave functions and iterative diagonalization of Hamiltonian. Because PWDFT.jl is implemented in Julia, matrix operations within which plane wave KSDFT are formulated, are particularly easy to be implemented as used. With these featuresPWDFT.jl is expected to be useful for for beginners KS-DFT implementers and researchers who want to implement their new methods quickly. PWDFT.jl is freely available at <https://github.com/f-fathurrahman/PWDFT.jl>.

Introduction

Blah blah

Main Objectives

- Lorem ipsum dolor sit amet, consectetur.
- Nullam at mi nisl. Vestibulum est purus, ultricies cursus volutpat sit amet, vestibulum eu.
- Praesent tortor libero, vulputate quis elementum a, iaculis.
- Phasellus a quam mauris, non varius mauris. Fusce tristique, enim tempor varius porta, elit purus commodo velit, pretium mattis ligula nisl nec ante.
- Ut adipiscing accumsan sapien, sit amet pretium.
- Estibulum est purus, ultricies cursus volutpat
- Nullam at mi nisl. Vestibulum est purus, ultricies cursus volutpat sit amet, vestibulum eu.
- Praesent tortor libero, vulputate quis elementum a, iaculis.

Materials and Methods

blah blah

Mathematical Section

blah blah

Results

Blah

Treatments	Response 1	Response 2
Treatment 1	0.0003262	0.562
Treatment 2	0.0015681	0.910
Treatment 3	0.0009271	0.296

Table 1: Table caption

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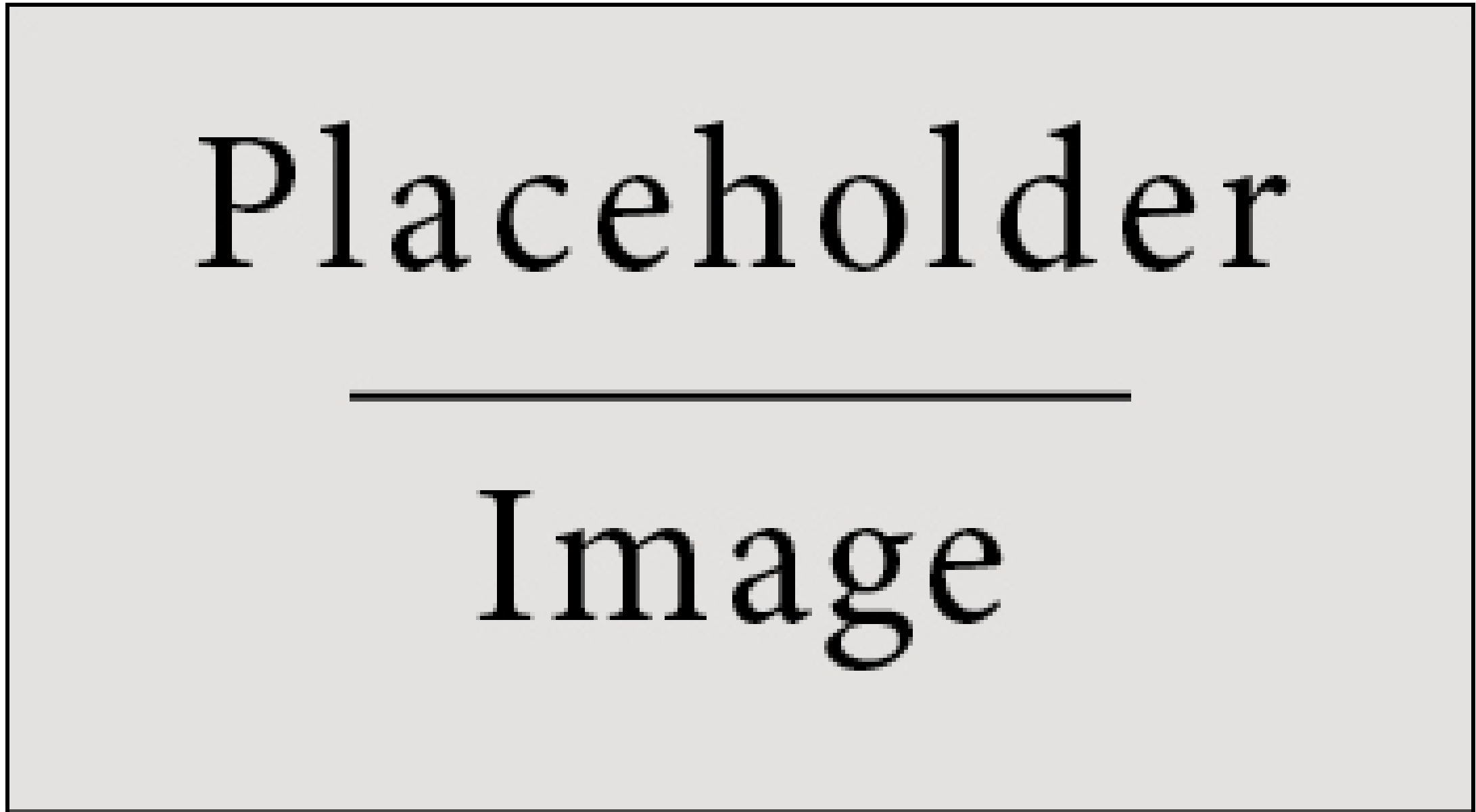


Figure 1: Figure caption

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Treatments	Response 1	Response 2
Treatment 1	0.0003262	0.562
Treatment 2	0.0015681	0.910
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Table 2: Table caption

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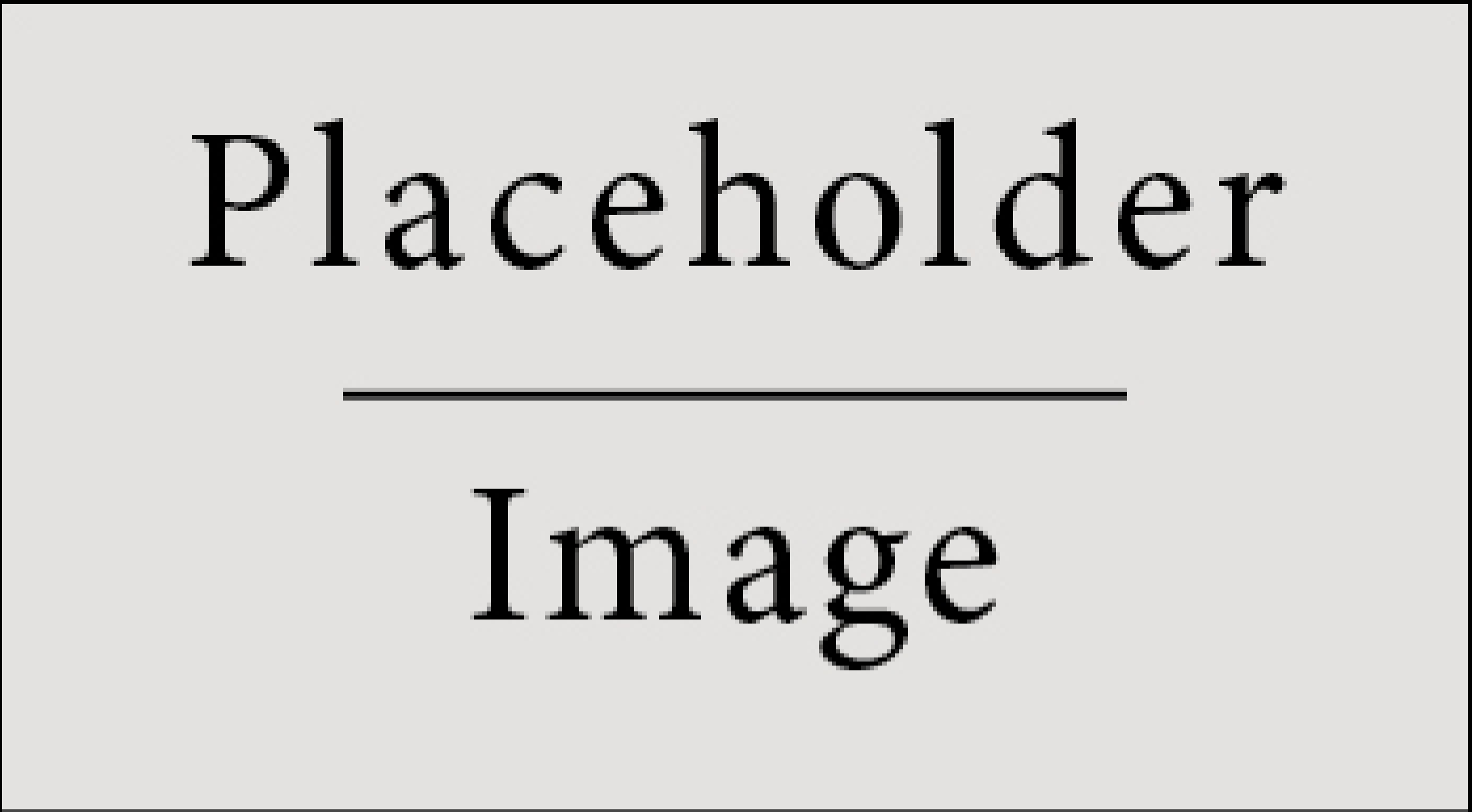


Figure 2: Figure caption

Conclusions

- Pellentesque eget orci eros. Fusce ultricies, tellus et pellentesque fringilla, ante massa luctus libero, quis tristique purus urna nec nibh. Phasellus fermentum rutrum elementum. Nam quis justo lectus.
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Forthcoming Research

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Acknowledgements

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