

[Thesis Title]

Thesis by
[Your Full Name]

In Partial Fulfillment of the Requirements for the
Degree of
[Name of Degree]

The Caltech logo, featuring the word "Caltech" in a bold, orange, sans-serif font.

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California

[Year Degree Conferred]
Defended [Exact Date]

© [Year Degree Conferred]

[Your Full Name]

ORCID: [Author ORCID]

All rights reserved

Choose one from
the choices in the
source code!! And
delete this todo
when you're done
that. :-)

ACKNOWLEDGEMENTS

[Add acknowledgements here. If you do not wish to add any to your thesis, you may simply add a blank titled Acknowledgements page.]

ABSTRACT

[This abstract must provide a succinct and informative condensation of your work. Candidates are welcome to prepare a lengthier abstract for inclusion in the dissertation, and provide a shorter one in the CaltechTHESIS record.]

TABLE OF CONTENTS

Acknowledgements	iii
Abstract	iv
Table of Contents	v
List of Illustrations	vi
List of Tables	vii
Chapter I: nomenclature	1
Chapter II: G_0W_0	2
2.1 Interpretive procedure	2
Chapter III: This is the Third Chapter	4
Chapter IV: This is the Fourth Chapter	5
Chapter V: This is the Fifth Chapter	6
Chapter VI: This is the Sixth Chapter	7
Chapter VII: This is the Seventh Chapter	8
Chapter VIII: This is the Eighth Chapter	9
Appendix A: Questionnaire	10
Appendix B: Consent Form	11
Pocket Material: Map of Case Study Solar Systems	

LIST OF ILLUSTRATIONS

*Number**Page*

LIST OF TABLES

*Number**Page*

Chapter 1

NOMENCLATURE

What follows is uses the restricted Hartree-Fock formalism with doubly occupied

	Symbol	Description
spatial orbitals.	i, j, k, l	Occupied orbitals
	a, b, c, d	Virtual orbitals
	p, q, r, s	General MO basis
	$\mu, \nu, \lambda, \sigma$	AO basis
	$(\mu\nu \lambda\sigma)$	Two-electron integrals

Chapter 2

G_0W_0

2.1 Interpretive procedure

The procedure that was used to compute the quasiparticle energies is given by the below equation:

$$\delta_{pq} F_{pq}^{HF} [\gamma^{DFT}] + \Sigma_p^{corr}(\varepsilon_p^{QP}) = \varepsilon_p^{QP} \quad (2.1)$$

We explain the notation starting from left to right. The first term corresponds to taking the diagonal δ_{pq} of the Hartree-Fock matrix F_{pq}^{HF} evaluated at a given electron density γ . These electron densities are obtained from a previous mean-field calculation, either γ_{DFT} or γ_{HF} . The second term evaluates the real part of the correlation self-energy for the ε_p^{QP} determined in the previous iteration. The right side of the equality gives the updated quasiparticle energy.

The Fock Matrix

In the basis of atomic orbitals, this is given by:

$$F_{\mu\nu}^{HF} = h_{\mu\nu} + \sum_{\lambda\sigma} P_{\lambda\sigma} (\mu\nu|\lambda\sigma) - \frac{1}{2} \sum_{\lambda\sigma} P_{\lambda\sigma} (\mu\lambda|\nu\sigma) \quad (2.2)$$

where $h_{\mu\nu}$ is the one-electron part of the Hamiltonian, $P_{\lambda\sigma}$ is the density matrix, and $(\mu\nu|\lambda\sigma)$ is one of the two-electron integrals. Cite Szabo. This is the simple form of the Hartree-Fock matrix that we want to use here and not the DFT Fock matrix. We transform this Fock matrix into the MO basis with:

$$F_{pq} = \sum_{\mu} \sum_{\nu} C_{\mu p}^* F_{\mu\nu} C_{\nu q} \quad (2.3)$$

where C is the matrix of MO coefficients. Another useful identity is for the density matrix in terms of the MO coefficients from the mean-field calculation:

$$P_{\mu\nu} = 2 \sum_{i=1}^{N/2} C_{\mu i} C_{\nu i}^* \quad (2.4)$$

We note that the sum runs only over the $N/2$ occupied *spatial* orbitals.

Real Correlation-Solve Energy

This is the second term in 2.1. It is dynamic, as opposed to the previous Fock term that was discussed, as it is updated with a new quasiparticle energy in each

iteration. In the case of the G_0W_0 approximation, we are only interested in the diagonal element of Σ^{corr} corresponding to the orbital with index p . This function is evaluated at the QP energy ε_p^{QP} just obtained in the previous iteration. We will go into greater detail about the form of Σ^{corr} in the next chapter.

*Chapter 3***THIS IS THE THIRD CHAPTER**

[You can have chapters that were published as part of your thesis. The text style of the body should be single column, as it was submitted to the publisher, not formatted as the publisher did.]

Chapter 4

THIS IS THE FOURTH CHAPTER

Chapter 5

THIS IS THE FIFTH CHAPTER

Chapter 6

THIS IS THE SIXTH CHAPTER

Chapter 7

THIS IS THE SEVENTH CHAPTER

Chapter 8

THIS IS THE EIGHTH CHAPTER

Appendix A

QUESTIONNAIRE

Appendix B

CONSENT FORM

POCKET MATERIAL: MAP OF CASE STUDY SOLAR
SYSTEMS