UNIVERSITY NAME

DOCTORAL THESIS

Thesis Title

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Declaration of Authorship

I, Asier RODRÍGUEZ ESCALANTE, declare that this thesis titled, "Thesis Title" and the work presented in it are my own. I confirm that:

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"Thanks to my solid academic training, today I can write hundreds of words on virtually any topic without possessing a shred of information, which is how I got a good job in journalism."

Dave Barry

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Abstract

Faculty Name
Department or School Name

Doctor of Philosophy

Thesis Title

by Asier RODRÍGUEZ ESCALANTE

The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

Acknowledgements

The acknowledgments and the people to thank go here, don't forget to include your project advisor...

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List of Abbreviations

NEGF	**N**on **E**quilibrium **G**reen's **F**unction
WSF	**W**hat (it) **S**tands **F**or

Physical Constants

Speed of Light $c_0 = 2.997\,924\,58 \times 10^8\,\mathrm{m\,s^{-1}}$ (exact)

List of Symbols

a	distance	m
P	power	W ($\mathrm{J\,s^{-1}}$)
ω	angular frequency	rad

For/Dedicated to/To my…

Chapter 1

Theoretical and computational tools

1.1 Density Functional Theory

Density-functional theory (DFT) is an approach to study the electronic structure of many-body problems, which allows the computational treatment large and complex systems. In fact, one of the reasons why DFT has become an essential tool in many areas of physics including condensed-matter theory is the increasing availability and power of computational processing. DFT is mainly based on the fact that any property of a system of many interacting particles can be viewed as a functional of the ground state density [**martin]. The famous paper by Hohenberg and Kohn in 1964 [** in martin] laid the groundwork of modern DFT, while the formulation presented in a 1965 paper by Kohn and Sham [** in martin] has prevailed as one of the most useful approaches up to this day. In the following subsections we will present the basics of this method, and then review a specific implementation, namely SIESTA, which will be used throughout this work.

1.1.1 Basics of DFT

The goal is to solve the many-body problem through Schrödinger's equation.

1.1.2 SIESTA

summary: In this method the effect of the core electrons is described by soft norm-conserving pseudopotentials and the electronic structure of the valence electrons is expanded in a basis set of numerical atomic orbitals with finite range

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