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

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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 Non Equilibrium Green's Function
WSF   What (it) Stands For

Physical Constants

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

List of Symbols

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

For/Dedicated to/To my…

Chapter 1

Theoretical and computational tools

1.1 DFT with SIESTA

Goal is to solve many-body problem through Schrödinger's equation.

1.1.1 Basics of DFT

1.1.2 SIESTA

summary: In this method the effect of the core electrons is described by soft norm-conserving pseudopotentials34 and the electronic structure of the valence electrons is expanded in a basis set of numerical atomic orbitals with finite range

1.2 Transport through NEGF

In this section the theory of nonequilibrium Green's functions (NEGF) will be presented, as the underlying theory of various programs that will be used (TRANSIESTA *** and TBRANS***) to study transport properties of the desired materials. Knowledge of (first- and second-quantized) quantum mechanics will be assumed, and the starting point will be an equilibrium state, which will lay the foundations and the basic properties of Green's functions. We will then delve into NEGF through the Keldysh formalism, and afterwards explore a simple and conceptually useful reformulation of this theory by S. Datta *et al***. Finally, we will overview the implementation in TRANSIESTA.

1.2.1 Equilibrium Green's functions

1.2.2 Keldysh formalism

1.2.3 TranSIESTA and TBtrans

1.2.4 sisl

Bibliography

[1]C. Moreno, M. Vilas-Varela, B. Kretz, A. Garcia-Lekue, M. V. Costache, M. Paradinas, M. Panighel, G. Ceballos, S. O. Valenzuela, D. Peña, and A. Mugarza, "Bottom-up synthesis of multifunctional nanoporous graphene", Science **360**, 199–203 (2018).