



## Simulating Correlations with Computers

Eva Pavarini and Erik Koch (Eds.)

Forschungszentrum Jülich GmbH  
Institute for Advanced Simulation

**Lecture Notes of the Autumn School on  
Correlated Electrons 2021**

Eva Pavarini and Erik Koch (Eds.)

## **Simulating Correlations with Computers**

Autumn School organized by  
the Institute for Advanced Simulation  
at Forschungszentrum Jülich  
20 – 24 September 2021

Schriften des Forschungszentrums Jülich  
Modeling and Simulation

Band / Volume 11

---

ISSN 2192-8525

ISBN 978-3-95806-529-1

# Contents

## Preface

1. Second Quantization and Jordan-Wigner Representations  
*Erik Koch*
2. Fundamentals of Quantum Chemistry  
*Klaus Doll*
3. Lies My Teacher Told Me About Density Functional Theory:  
Seeing Through Them with the Hubbard Dimer  
*Kieron Burke*
4. Hubbard Dimer in GW and Beyond  
*Pina Romaniello*
5. Dynamical Mean-Field Theory for Materials  
*Eva Pavarini*
6. Green Functions and Self-Energy Functionals  
*Robert Eder*
7. Green Functions in the Renormalized Many-Body Perturbation Theory  
*Václav Janiš*
8. An Essential Introduction to NEGF Methods for Real-Time Simulations  
*Gianluca Stefanucci*
9. Orbital Entanglement and Correlation  
*Christian Schilling*
10. Analog Quantum Simulations of the Hubbard Model  
*Walter Hofstetter*
11. Programming Quantum Computers  
*Kristel Michielsen*
12. Quantum Chemistry on Quantum Computers  
*Libor Veis*
13. Quantum Computing – Quo Vadis?  
*David DiVincenzo*

## Index