

Cover Page



Universiteit Leiden



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**Author:** Eisenmayer, Thomas J.

**Title:** Coherent dynamics in solar energy transduction

**Issue Date:** 2014-12-15

# Curriculum Vitae



## Education

PERIOD 2010 — 2014 Leiden Institute of Chemistry

PhD. Computational Quantum Mechanics

Supervised by Dr. F. Buda and Prof. Dr. H.J.M. de Groot.

**Title:** *Coherent Dynamics in Solar Energy Transduction.*

PERIOD 2007 — 2010 Leiden University

MSc. Physical & Theoretical Chemistry

Thesis with Dr. F. Buda and Prof. Dr. H.J.M. de Groot  
(grade for thesis: 10).

**Thesis subject:** *Asymmetry in Reaction Centers.*

**Extra-curricular:** Honours Class, Science Based Business.

**Certificate:** Financial Markets Summer School, London  
School of Economics (2009).

PERIOD 2002 — 2007 Delft University of Technology

BSc. Molecular Science and Technology

Thesis with Prof. Dr. L.D.A. Siebbeles and Dr. J.M. Schins  
(grade for thesis: 10).

**Thesis subject:** *Excited State and Charge Photogeneration  
Dynamics in P3HT and P3HT/PCBM blends.*

**Majors:** Molecular Quantum Mechanics, Physical Chemistry.

**Minors:** Economics, Sustainable Energy.

PERIOD 2001 — 2002 Delft University of Technology

Technology, Policy and Management

→ Propedeutic exam.

PERIOD 1994 — 2000 Sint Ignatius Gymnasium

## Languages

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ENGLISH	Native
DUTCH	Native
ITALIAN	Fluent

GERMAN	Proficient
FRENCH	Basic

## Programming & Software

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Fortran Bash Unix Matlab Igor Pro LaTeX

OCTOPUS CPMD Gaussian Amsterdam Density Functional

## Conference Proceedings

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- Thomas J. Eisenmayer, Huub J. M. de Groot, Francesco Buda. *Real-Time Simulations of Photoinduced Processes*, CHAINS, (Veldhoven, 2014). [Talk](#)
- Thomas J. Eisenmayer, Huub J. M. de Groot, Francesco Buda. *Charge Transfer and Coherent Dynamics*, Physics@FOM, (Veldhoven, 2014). [Talk](#)
- Thomas J. Eisenmayer, Huub J. M. de Groot, Francesco Buda. *From Photosynthesis to Solar Fuel*, Holland Research School of Molecular Chemistry, (Naturalis, 2013). [Talk](#)
- Thomas J. Eisenmayer, A. Monti, J. Rombouts, Huub J. M. de Groot, Francesco Buda. *In Silico Design of Novel Charge Separators*, European Science Foundation, (Torun, 2013). [Talk](#)
- Thomas J. Eisenmayer, Huub J. M. de Groot, J. Neugebauer, Francesco Buda. *Mechanism and Reaction Coordinate of Directional Charge Separation in Bacterial Reaction Centers*, Study group Spectroscopy and Theory, (Utrecht, 2012). [Talk](#)
- Jorge Piris, Thomas J. Eisenmayer, Minh T. Trinh, Juleon M. Schins and Laurens D.A. Siebbeles: *Photoexcitations and Charge Generation Dynamics in P3HT/PCBM Blended Films Studied by Ultrafast Transient Absorption Spectroscopy*. Materials Research Society, Symposium H: Nanostructured Solar Cells (Boston, 2007). [Abstract](#)



## List of Publications

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- T. J. Eisenmayer, F. Buda. "Real-Time Simulations of Photoinduced Coherent Charge Transfer and Proton-Coupled Electron Transfer", *ChemPhysChem*, 2014, 15 (15), pp 3258-3263.  
DOI: 10.1002/cphc.201402444  
--> **Chapters 5 and 7** of this thesis.
  
- T. J. Eisenmayer, H. J. M. de Groot, E. van de Wetering, J. Neugebauer, F. Buda, "Mechanism and Reaction Coordinate of Directional Charge Separation in Bacterial Reaction Centers", *Journal of Physical Chemistry Letters*, 2012, 3, pp 694-697.  
DOI: 10.1021/jz201695p  
--> **Chapter 3** of this thesis.
  
- T. J. Eisenmayer, J. A. Lasave, A. Monti, H. J. M. de Groot, F. Buda, "Proton Displacements Coupled to Primary Electron Transfer in the Rhodobacter Sphaeroides Reaction Center", *Journal of Physical Chemistry B*, 2013, 38, pp 11162-11168.  
DOI: 10.1021/jp401195t  
--> **Chapter 4** of this thesis.
  
- K. S. Joya, J. L. Valles-Pardo, Y. F. Joya, T. J. Eisenmayer, B. Thomas, F. Buda, H. J. M. de Groot, "Molecular Catalytic Assemblies for Electro-driven Water Splitting", 2013, *ChemPlusChem*, 78, pp 35-47.  
DOI: 10.1002/cplu.201200161
  
- T. J. Eisenmayer, J. Marcelis, H. J. M. de Groot and F. Buda, 2014, "Redox levels and Oxidation Potential in Photosystem II: A DFT investigation", *to be submitted*.  
--> **Chapter 6** of this thesis.
  
- 2015, "A Practical Quantum Theory for Efficient Solar Energy Transduction", *in preparation*.  
--> **Outlook** of this thesis.