

# Thijs Stuyver – Curriculum Vitae

## PERSONAL DETAILS

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Citizenship: Belgian

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## SCIENTIFIC QUALIFICATIONS

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### Work Experience

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|---|-------------------------|
| Junior professor at Ecole National Supérieure de Chimie de Paris (ENSCP) – PSL University   | 01/01/2023 - now        |
| Postdoctoral researcher at the Massachusetts Institute of Technology (MIT) in the research group of Professor C. Coley                  | 25/04/2021 – 31/12/2022 |
| Postdoctoral researcher at the Institute of Chemistry of The Hebrew University of Jerusalem in the research group of Professor S. Shaik | 01/09/2020 – 24/04/2021 |
| Postdoctoral research fellow of the Research Foundation Flanders (FWO)  | 01/10/2018 – 31/08/2020 |

### Education

#### Vrije Universiteit Brussel

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| ➤ PhD in Sciences – Chemistry  | 01/10/2014 – 30/05/2018 |
| ➤ Master of Science in Management<br><i>magna cum laude</i>  | 21/09/2015 – 07/07/2018 |
| ➤ Master of Science in Chemistry<br>Cluster: Molecular and macromolecular design<br><i>summa cum laude</i> | 24/09/2012 – 06/07/2014 |
| ➤ Bachelor of Science in Chemistry<br><i>summa cum laude</i>   | 22/09/2009 – 07/07/2012 |

#### DVM Humaniora Aalst

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| ➤ Sciences-Mathematics | 01/09/2003 – 30/06/2009 |
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### Scholarships and Grants

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| ➤ Swiss Government Excellence Scholarship awarded by the Swiss Federal Commission for Scholarships for Foreign Students | 25/03/2021 |
| • Project title: <i>Reaction network exploration through chemical concepts</i>  |            |

- Marie Skłodowska-Curie Action – Individual Fellowship awarded by the European Commission 08/02/2021
  - Project title: *Reaction network exploration through chemical concepts*
- Research Foundation Flanders (FWO) long-term travel grant awarded, 19.800 euro 12/11/2018
- Postdoctoral fellowship awarded by Research Foundation Flanders (FWO) 27/06/2018
  - Project title: *Reactivity and transport properties of (di)radical(oid)s: A combined valence bond and conceptual DFT study*
- Research Foundation Flanders (FWO) short-term travel grant awarded 07/07/2017
- Research Foundation Flanders (FWO) long-term travel grant awarded 22/03/2016
- PhD scholarship awarded by Research Foundation Flanders (FWO) 25/06/2014
  - Project title: *Qualitative insights into conduction in molecular electronic devices using the Source-and-sink potential method and density functional theory based chemical concepts*

#### **Distinctions, Honors and Awards**

- Invited speaker at the conference “World Association of Theoretical and Computational Chemists” (WATOC) 2020-2022 in Vancouver, Canada 03/07/2022 – 08/07/2022
- Winner of the I. Vanderschueren prize, awarded for the most commendable PhD thesis in the physical sciences and engineering defended at the Vrije Universiteit Brussel between 2012 and 2019 (20.000 euro) 25/09/2020
- Invited speaker at the conference “Gathering on Transport at the Nanoscale” at Centro Internacional de Ciencias, Cuernavaca, Mexico 29/10/2018 – 09/11/2018
- Winner of the award for the best oral presentation in the session on Physical and Theoretical Chemistry at “ChemCYS 2018”, Blankenberge, Belgium 21/02/2018 – 23/02/2018
- Invited speaker at the conference “Conference on Transport at the Nanoscale” at Centro Internacional de Ciencias, Cuernavaca, Mexico 25/11/2017 – 29/11/2017
- Selected Speaker at the Solvay Conference “Conceptual Quantum Chemistry: Present Aspects and Challenges for the Future”, at Université Libre de Bruxelles, Brussels, Belgium 04/04/2016 – 08/04/2016

- Winner of the Royal Chemical Society Flanders (KVCV) prize for the most commendable student graduating in Chemistry in 2014 12/12/2014

### Research Stays and Study Visits

- Long term research stay with Professor Sason Shaik at The Hebrew University, Jerusalem, Israel 01/10/2018 – 31/08/2020
- Short study visit with Professor Roald Hoffmann at Cornell University, Ithaca, NY, USA 25/03/2018 – 17/04/2018
- Short study visit with Professor Roald Hoffmann at Cornell University, Ithaca, NY, USA 06/02/2017 – 19/02/2017
- Research stay with Professor Roald Hoffmann at Cornell University, Ithaca, NY, USA 27/05/2016 – 02/08/2016
- Short study visit with Professor Patrick W. Fowler at the University of Sheffield, Sheffield, UK 25/04/2016 – 29/04/2016
- Short study visit with Sylvain Latil at the CEA in Paris, France 25/05/2015 – 29/05/2015

### Research and Publications

#### *Journal publications:*

- Voltage-driven control of single-molecule keto-enol equilibrium in a two-terminal junction system, C. Tang, T. Stuyver, T. Lu, J. Liu, Y. Ye, T. Gao, L. Lin, J. Zheng, W. Liu, J. Shi, S. Shaik\*, H. Xia\*, W. Hong\*, *Nat. Commun.* **2023**, 3657.
- Machine learning-guided computational screening of new candidate reactions with high bioorthogonal click potential, T. Stuyver\*, C. Coley\*, *Chem. Eur. J.* **2023**, e202300387.
- Reaction profiles for quantum chemistry-computed [3+2] cycloaddition reactions, T. Stuyver, K. Jorner, C. Coley\*, *Sci. Data* **2023**, 10, 66.
- QMugs 1.1: Quantum mechanical properties of organic compounds commonly encountered in reactivity datasets, R. Neeser, C. Isert, T. Stuyver, G. Schneider\*, C. Coley\*, *Chem. Data Collect.* **2023**, 46, 101040.
- Predictive chemistry: machine learning for reaction deployment, reaction development, and reaction discovery, Z. Tu, T. Stuyver, C. Coley\*, *Chem. Sci.* **2023**, 14, 226-244.
- Local Electric Fields: From Enzyme Catalysis to Synthetic Catalyst Design, K. D. Dubey\*, T. Stuyver\*, S. Shaik\*, *J. Phys. Chem. B* **2022**, 126, 10285-10294.
- Quantum chemistry-augmented neural networks for reactivity prediction: performance generalizability and interpretability, T. Stuyver, C. Coley\*, *J. Chem. Phys.* 2022, **156**, 084104.
- Can the philicity of radicals be influenced by oriented external electric fields?, R. Van Lommel\*, R. H. Verschueren, W. M. De Borggraeve, F. De Vleeschouwer, T. Stuyver\*, *Org. Lett.* 2022, **24**, 1-5.
- Evidence for new enantiospecific interaction force in chiral biomolecules, Y. Kapon, A. Saha, T. Duanis-Assaf, T. Stuyver, A. Ziv, T. Metzger, S. Yochelis, S. Shaik\*, R. Namaan\*, M. Reches\*, Y. Paltiel\*, *Chem* 2021, **7**, 2787-2799.
- Resolving entangled reactivity modes through external electric fields and substitution: Applications to E2/SN2 reactions, T. Stuyver\*, S. Shaik\*, *J. Org. Chem.* 2021, **86**, 9030-9039.
- Promotion energy analysis predicts reaction modes: Nucleophilic and electrophilic aromatic substitution reactions, T. Stuyver\*, S. Shaik\*, *J. Am. Chem. Soc.* 2021, **143**, 4367-4378.
- Modulating the radical reactivity of phenyl radicals with the help of distonic charges: it is all about electrostatic catalysis, T. Mondal, S. Shaik\*, H. Kenttämaa, T. Stuyver\*, *Chem. Sci.* 2021, **12**, 4800-4809.

- Single-molecule conductance in a unique cross-conjugated tetra(aminoaryl)ethene, S. M. Rivero, P. G. Arroyo, L. Li, S. Gunasekaran, T. Stuyver, M. J. Mancheño, M. Alonso\*, L. Venkataraman\*, J. L. Segura\*, J. Casado\*, *Chem. Commun.* 2021, **57**, 591-594.
- Extending conceptual DFT to include additional variables: oriented external electric field, T. Clarys, T. Stuyver, F. De Proft\*, P. Geerlings, *Phys. Chem. Chem. Phys.* 2021, **23**, 990-1005.
- Unifying conceptual density functional and valence bond theory: the hardness-softness conundrum associated with protonation reactions and uncovering complementary reactivity modes, T. Stuyver\*, S. Shaik\*, *J. Am. Chem. Soc.* 2020, **142**, 20002-20013.
- Electric-field mediated chemistry: uncovering and exploiting the potential of (oriented) electric fields to exert chemical catalysis and reaction control, S. Shaik\*, D. Danovich, J. Joy, Z. Wang, T. Stuyver\*, *J. Am. Chem. Soc.*, 2020, **142**, 12551-12562.
- How do local reactivity descriptors shape the potential energy surface associated with chemical reactions? The valence bond delocalization perspective, T. Stuyver\*, F. De Proft, P. Geerlings, S. Shaik\*, *J. Am. Chem. Soc.*, 2020, **142**, 10102-10113.
- Solvent-organization and rate-regulation of a Menshutkin reaction by oriented-external electric fields are revealed by combined MD and QM/MM calculations, K. D. Dubey\*, T. Stuyver\*, S. Kalita, S. Shaik\*, *J. Am. Chem. Soc.*, 2020, **142**, 9955-9965 (*shared co-first authorship*).
- Oriented (local) electric fields drive the millionfold enhancement of the H-abstraction catalysis observed for synthetic metalloenzyme analogues, T. Stuyver\*, R. Ramanan, D. Mallick, S. Shaik\*, *Angew. Chem., Int. Ed.*, 2020, **59**, 7915-7920.
- Oriented external electric fields and ionic additives elicit catalysis and mechanistic crossover in oxidative addition reactions, J. Joy\*, T. Stuyver, S. Shaik\*, *J. Am. Chem. Soc.*, 2020, **142**, 3836-3850.
- TITAN: a code for modeling and generating electric fields – features and applications to enzymatic reactivity, T. Stuyver\*, J. Huang, D. Mallick, D. Danovich, S. Shaik\*, *J. Comput. Chem.*, 2020, **41**, 74-82.
- External electric field effects on chemical structure and reactivity, T. Stuyver, D. Danovich, J. Jyothish, S. Shaik\*, *WIREs: Comput. Mol. Sci.*, 2019, **10**, e1438.
- Do diradicals behave like radicals?, T. Stuyver, B. Chen, T. Zeng, P. Geerlings, F. De Proft, R. Hoffmann\*, *Chem. Rev.* 2019, **119**, 11291-11351.
- Captodative substitution enhances the diradical character of compounds, reduces aromaticity and controls single molecule conductivity patterns: a valence bond study, T. Stuyver\*, D. Danovich, S. Shaik\*, *J. Phys. Chem. A*, 2019, **123**, 7133-7141 (*part of the Paul Geerlings festschrift*).
- Global and local aromaticity of acenes from the information-theoretic approach in density functional reactivity theory, D. Yu, T. Stuyver, C. Rong\*, M. Alonso, T. Lu, F. De Proft\*, P. Geerlings\*, S. Liu\*, *Phys. Chem. Chem. Phys.*, 2019, **21**, 18195-18210.
- Electrophilic aromatic substitution reactions: mechanistic landscape, electrostatic and electric-field control of reaction rates and mechanistic crossovers, T. Stuyver\*, D. Danovich, F. De Proft, S. Shaik\*, *J. Am. Chem. Soc.*, 2019, **141**, 9719-9730.
- Cross conjugation in polyenes and related hydrocarbons: what can be learned from valence bond theory about single-molecule conductance?, J. Gu, W. Wu\*, T. Stuyver\*, D. Danovich, R. Hoffmann\*, Y. Tsuji, S. Shaik\*, *J. Am. Chem. Soc.*, 2019, **141**, 6030-6047.
- Insights into the trends in the acidity strength of organic and inorganic compounds: a valence bond perspective, T. Stuyver\*, D. Danovich, S. Shaik\*, *J. Phys. Chem. A*, 2019, **123**, 1851-1860.
- Diradical character as a guiding principle for the insightful design of molecular nanowires with an increasing conductance with length, T. Stuyver\*, T. Zeng, Y. Tsuji, P. Geerlings, F. De Proft, *Nano Lett.*, 2018, **18**, 7298-7304.
- Towards the design of bithermoelectric switches, T. Stuyver\*, P. Geerlings, F. De Proft, M. Alonso, *J. Phys. Chem. C*, 2018, **122**, 24436-24444.
- Qualitative insights into the transport properties of Hückel/Möbius (anti-)aromatic compounds: Application to expanded porphyrins, T. Stuyver\*, S. Fias, P. Geerlings, F. De Proft, M. Alonso, *J. Phys. Chem. C*, 2018, **122**, 19842-19856 (*featured on the cover*).

- Captodative substitution: A strategy for enhancing the conductivity of molecular electronic devices, T. Stuyver, T. Zeng, Y. Tsuji, S. Fias, P. Geerlings, F. De Proft\*, *J. Phys. Chem. C*, 2018, **122**, 3194-3200 (*featured on the cover*).
- Conductance switching in expanded porphyrins through aromaticity and topology changes, T. Stuyver, M. Perrin, P. Geerlings, F. De Proft, M. Alonso\*, *J. Am. Chem. Soc.*, 2018, **140**, 1313-1326.
- Extension of the source-sink potential approach to Hartree Fock and Density Functional Theory: a new tool to visualize the ballistic current through molecules, S. Fias\*, T. Stuyver, *J. Chem. Phys.*, 2017, **147**, 184102.
- Exploring electrical currents through nanographenes: Visualization and tuning of the through-bond transmission paths, T. Stuyver\*, N. Blotwijk, S. Fias, F. De Proft, P. Geerlings, *ChemPhysChem*, 2017, **18**, 3012.
- Dioxygen: What makes this triplet diradical kinetically persistent?, W.T. Borden\*, R. Hoffmann\*, T. Stuyver, B. Chen, *J. Am. Chem. Soc.*, 2017, **139**, 9010-9018 (*editor's choice*).
- The influence of linkers on quantum interference: A linker theorem, Y. Tsuji\*, T. Stuyver, S. Gunasekaran, L. Venkataraman, *J. Phys. Chem. C*, 2017, **121**, 092310.
- Enhancing the conductivity of molecular electronic devices, T. Stuyver\*, S. Fias, F. De Proft, P. Geerlings, Y. Tsuji, R. Hoffmann, *J. Chem. Phys.*, 2017, **146**, 092310.
- Back of the envelope selection rule for molecular transmission: A curly arrow approach, T. Stuyver, S. Fias, F. De Proft, P. Geerlings\*, *J. Phys. Chem. C*, 2015, **119**, 26390-26400.
- The relation between delocalization, long bond order structure count and transmission: An application to molecular wires, T. Stuyver\*, S. Fias, F. De Proft, P. Geerlings, *Chem. Phys. Lett.*, 2015, **142**, 092310.
- Conduction of molecular electronic devices: Qualitative insights through atom-atom polarizabilities, T. Stuyver\*, S. Fias\*, F. De Proft, P. W. Fowler, P. Geerlings, *J. Chem. Phys.*, 2015, **142**, 094103.
- Analysis of aromaticity in planar metal systems using the linear response kernel, S. Fias\*, Z. Boisdenghien, T. Stuyver, M. Audiffred, G. Merino, P. Geerlings, F. De Proft\*, *J. Phys. Chem. A*, 2013, **117**, 3556.

#### Book chapters:

- Electrophilic aromatic substitution: from isolated reactant approaches to chemical reactivity in solvent, R. Van Lommel, P. Geerlings, T. Stuyver, S. Moors, F. De Proft, In *Chemical Reactivity*, Eds: S. Kaya, L. von Szentpaly, G. Serdaroglu, L. Guo, Elsevier, 2023.
- Bridging conceptual density functional and valence bond theories, T. Stuyver, S. Shaik, In *Conceptual Density Functional Theory: Towards a New Chemical Reactivity Theory*, Eds: S. Liu, Wiley, 2022.
- A tutorial on XMVB, F. Ying, C. Zhou, A. Shurki, D. Danovich, T. Stuyver, B. Braïda, W. Wu, In *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, Elsevier, 2022.
- The impact of electric fields on chemical structure and reactivity, S. Shaik, D. Danovich, K. D. Dubey, T. Stuyver, In *Effects of electric fields on structure and reactivity: New horizons in chemistry*, Eds: S. Shaik, T. Stuyver, Royal Society of Chemistry Publishing: London, 2021.
- Computational generation and quantification of electric fields and electrostatics-mediated catalyst optimization, T. Stuyver, J. Joy, D. Danovich, S. Shaik, In *Effects of electric fields on structure and reactivity: New horizons in chemistry*, Eds: S. Shaik, T. Stuyver, Royal Society of Chemistry Publishing: London, 2021.
- New insights and horizons from the linear response function in conceptual DFT, P. Geerlings, S. Fias, T. Stuyver, P. Ayers, R. Balawender, F. De Proft, in *Density Functional Theory*, Ed: by D. Glossman-Mitnik, IntechOpen, 2019.

*Edited books:*

Effects of electric fields on structure and reactivity: New horizons in chemistry, Eds: S. Shaik, T. Stuyver, Royal Society of Chemistry Publishing: London, 2021 (ISBN: 978-1-83916-169-8).

*Conference presentations:*

- **American Chemical Society (ACS) Fall Meeting 2022**, August 21 – August 25, 2022, Chicago (USA); T. Stuyver, C. Coley, Improving the performance, generalizability and explainability of neural networks for reactivity prediction through quantum chemistry-augmentation – oral presentation
- **World Association of Theoretical and Computational Chemists (WATOC) 2020**, July 3 – July 8, 2022, Vancouver (Canada); T. Stuyver, C. Coley, “Performance, generalizability and explainability of quantum chemistry-augmented neural networks for reactivity prediction” – oral presentation
- **Gathering on Transport at the Nanoscale**, October 29 – November 9, 2018, Cuernavaca (Mexico); T. Stuyver, P. Geerlings, F. De Proft, “Qualitative insights into the transport properties of molecular electronic devices: Diradical character as a guiding principle for the insightful design of molecular nanowires with an increasing conductance with length” – oral presentation
- **Quantum Chemistry in Belgium**, March 30, 2018, Brussels (Belgium); T. Stuyver, S. Fias, F. De Proft, P. Geerlings, “Qualitative insights into molecular conduction.” – oral presentation
- **ChemCYS**, February 21 – 23, 2018, Blankenberge (Belgium); T. Stuyver, S. Fias, F. De Proft, P. Geerlings, “Captodative substitution: A strategy for enhancing the conductivity of molecular electronic devices” – oral presentation
- **Conference on Transport at the Nanoscale**, November 25 – 29, 2017, Cuernavaca (Mexico); T. Stuyver, S. Fias, P. Geerlings, F. De Proft, “Exploring electrical currents through nanographenes: Visualization and tuning of the through-bond transmission paths” – oral presentation
- **EMN Meeting on Carbon Nanomaterials**, February 19 - 23, 2017, Orlando, FL (USA); T. Stuyver, S. Fias, P. Geerlings, F. De Proft, “Qualitative insights into the transport properties of carbon nanomaterials” – oral presentation
- **ChemCYS**, March 16 – 18, 2016, Blankenberge (Belgium); T. Stuyver, S. Fias, F. De Proft, P. Geerlings, “Qualitative insights into molecular conduction: A curly arrow rule” – oral presentation
- **Conceptual Quantum Chemistry: Present Aspects and Challenges for the Future**, April 4 – 8, 2016, Brussels (Belgium); T. Stuyver, S. Fias, P. Geerlings, F. De Proft, “Qualitative insights into molecular transmission: A curly arrow rule” – oral presentation
- **EMN Meeting on Theory and Computation**, November 9 – 12, 2015, Istanbul (Turkey); T. Stuyver, S. Fias, P. Geerlings, F. De Proft, “Insights into molecular transmission” – oral presentation
- **European Conference on Molecular Electronics**, September 1 – 5, 2015, Strasbourg (France); T. Stuyver, S. Fias, P. Geerlings, F. De Proft, “Qualitative insights into molecular transmission” – poster presentation

**Teaching Responsibilities**

- Teaching assistant during laboratory sessions for the first bachelor course “General Chemistry” at the Vrije Universiteit Brussel (15 ECTS; 25 students; 60 hours per year) 01/10/2014 – 07/07/2018
- Teaching of the exercise sessions for the second bachelor course “Introduction to Quantum Chemistry” at the Vrije Universiteit Brussel (3 ECTS; 12 students; 20 hours per year) 21/09/2015 – 07/07/2018
- Supervision of the bachelor thesis “Exploring Electrical Currents through Aromatic Hydrocarbons” by Nathalie Blotwijk 13/02/2017 – 17/09/2017
- Supervision of the bachelor thesis “Influence of an Electric Field on Chemical Properties and Overall Reactivity: A Conceptual and Computational Quantum Chemistry Approach” by Tom Clarys 07/02/2020 – 30/06/2020
- Supervision of the master thesis “Influence of an Electric Field on the Behavior of the Green Fluorescent Protein Chromophore: A Quantum Chemical Approach” by Tom Clarys 07/02/2021 – 30/06/2021

#### **Organization of international conferences**

- Member of the organizing committee of the one-day symposium, “Chemical Bonding in the 21<sup>st</sup> Century”, in honor of Prof. Roald Hoffmann (Brussels, Belgium) 28/05/2018

#### **ADMINISTRATIVE DUTIES AND LEADERSHIP**

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- Personnel representative of the Faculty of Sciences in the University Council of the Vrije Universiteit Brussel 25/09/2017 – 16/09/2018
- Personnel representative of the Faculty of Sciences in the Academic Council of the Vrije Universiteit Brussel 25/09/2017 – 16/09/2018
- Personnel representative of the Faculty of Sciences in the Education Council of the Vrije Universiteit Brussel 26/09/2016 – 17/09/2017
- Member of the educational assessment panel for the evaluation of the Erasmus Mundus Master in Theoretical Chemistry and Computational Modeling (TCCM) at KULeuven, Belgium 08/02/2016 – 30/05/2016
- Coordinator Education of the Student Council of the Vrije Universiteit Brussel 21/09/2015 – 12/09/2016
- University-wide student representative in the Education Council of the Vrije Universiteit Brussel 21/09/2015 – 12/09/2016
- Student representative of the Faculty of Sciences in the Education Council of the Vrije Universiteit Brussel 22/09/2014 – 14/09/2015
- Member of the board of the student association “Wetenschappelijke Kring”, responsible for the organization of events 27/09/2010 – 14/09/2014

## PROFESSIONAL SKILLS

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### **Languages**

- Dutch: native proficiency
- English: full professional proficiency
- French: working proficiency
- German: elementary proficiency
- Swedish: elementary proficiency
- Hebrew: elementary proficiency

### **Computational Skills**

- Advanced Python and elementary C++ programming, as well as Bash scripting
- Knowledge of quantum chemistry software: Gaussian09, ADF, Artaios, Molpro, Gamess-US, XMVB, Entos, autodE
- Knowledge of machine learning software and libraries: Tensorflow (Keras), PyTorch, Scikit-learn