

Thijs Stuyver – Curriculum Vitae

PERSONAL DETAILS

Citizenship: Belgian

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SCIENTIFIC QUALIFICATIONS

Work Experience

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

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

DVM Humaniora Aalst

- Sciences-Mathematics 01/09/2003 – 30/06/2009

Scholarships and Grants

- PR[AI]RIE-PSAI PhD grant (€140.000) 05/06/2026
- ChemAI PhD grant (€125.000) 25/05/2026

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| ➤ JCJC grant by Agence National de Recherche (ANR)
<i>(research funding to hire non-permanent research staff and to buy equipment – €330.000)</i> | 01/10/2024 |
| ➤ Major Research Program of PSL University: Artificial intelligence for chemistry – ChemAI <i>(coordinator of a university-wide project to implement AI and automation across the chemistry and chemical engineering departments – €2.100.000)</i> | 01/06/2024 |
| ➤ Start-up grant by Agence National de Recherche (ANR) and Centre National de Recherche Scientifique (CNRS)
<i>(research funding to hire non-permanent research staff and to buy equipment, amounting to €370.000 in total)</i> | 01/01/2023 |
| ➤ Swiss Government Excellence Scholarship awarded by the Swiss Federal Commission for Scholarships for Foreign Students <i>(personal research funding for 1 year – approximately €40.000; declined due to alternative job opportunity)</i> | 25/03/2021 |
| ➤ Marie Skłodowska-Curie Action – Individual Fellowship awarded by the European Commission <i>(personal research funding for 2 years – approximately €190.000; declined due to alternative job opportunity)</i> | 08/02/2021 |
| ➤ Research Foundation Flanders (FWO) long-term travel grant awarded (€19.800) | 12/11/2018 |
| ➤ Postdoctoral fellowship awarded by Research Foundation Flanders <i>(personal research funding for 3 years – approximately €180.000)</i> | 27/06/2018 |
| ➤ 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 <i>(personal research funding for 4 years – approximately €120.000)</i> | 25/06/2014 |

Distinctions, Honors and Awards

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| ➤ Fellow of the Paris School of AI, PR[AI]RIE-PSAI | 01/01/2025 – now |
| ➤ 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 | 25/09/2020 |

and engineering defended at the Vrije Universiteit Brussel between 2012 and 2019 (€20.000)

- 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 Supervision

PhD students:

- Javier Alfonso-Ramos (primary supervisor; defended February 2026) 01/03/2023 – 28/02/2026
- Bowen Deng (primary supervisor, ongoing) 01/02/2024 – now
- Basile Parmeli (co-supervised with Gilles Gasser, ongoing) 01/10/2024 – now
- Emilien Chen (primary supervisor, ongoing) 01/11/2024 – now
- Marie Wadih (co-supervised with Renaud Nicolaÿ) 01/10/2026 – now

Postdoctoral researchers:

- Maxime Ferrer 01/11/2024 – now
- Javier Alfonso-Ramos 01/04/2026 – now

Research engineers:

- Maximilian Fleck 30/05/2025 – now

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

Entrepreneurship and Technology Transfer

- Scientific co-founder, Plaskimia (<https://www.plaskimia.com/>) 2026 – now
 - Co-founded a company focused on plasma-activated microfluidic synthesis
 - Scientific lead for AI-driven reaction optimization and modelling

Research and Publications

Journal publications:

- Modelling reaction feasibility to identify new opportunities for sigmatropic rearrangements, J. P. Liles, N. Casetti, T. Stuyver*, C. Coley*, *ChemRxiv preprint*, **2026**, DOI: 10.26434/chemrxiv.15008353/v1.
- On-demand generation of COCl₂ through the oxidation of chloroform via non-thermal plasma in flow. F. Bruel, A. Favre-Reguillon, G. Morand*, S. Ognier, O. Venier, A. Bonn, T. Stuyver, M. Tatouliau, *Chem. Eng. J.* **2026** (under review).
- Predictive modelling enables exploration of the anticancer potential of Ruthenium (II) polypyridyl complexes. B. Parmelli, I. Vanlaeys, O. Blacque, P. Mesdom, K. Cariou, G. Gasser, T. Stuyver*, *ChemRxiv preprint*, **2026**, DOI: 10.26434/chemrxiv.15000025/v4.
- Robust transfer learning for Bayesian optimization of chemical reactions, G. Chen, M. Fleck, T. Stuyver*, *Digit. Discov.* **2026**, DOI: 10.1039/d6dd00527f.
- Reaction enumeration based on NBO-informed molecular graphs. J. E. Alfonso-Ramos, T. Stuyver*, *J. Comput. Chem.* **2026**, *47*, e70462.
- Leveraging hidden-space representations effectively in Bayesian optimization for experiment design through dimension-aware hyperpriors. G. Chen, M. Fleck, T. Stuyver*, *J. Chem. Theory Comput.* **2026**, *22*, 5594-5608.
- Revisiting the maximum hardness principle: A quantitative analysis on reaction datasets. A. Bajaj, F. Heidar-Zadeh, T. Stuyver, S. Habershon, P. W. Ayers, F. De Proft*, *J. Comput. Chem.* **2026**, *47*, e70365.
- Screening Diels–Alder reaction space to identify candidate reactions for self-healing polymer applications. M. Ferrer, B. Deng, J. E. Alfonso-Ramos, T. Stuyver*, *Digit. Discov.* **2025**, *4*, 3400-3410.
- Harnessing Surrogate Models for Data-efficient Predictive Chemistry: Descriptors vs. Learned Hidden Representations. G. Chen, T. Stuyver*, *Digit. Discov.* **2025**, *4*, 3227-3237.
- CYCLO70: A New Challenging Pericyclic Benchmarking Set for Kinetics and Thermochemistry Evaluation. J. E. Alfonso-Ramos, C. Adamo, E. Brémond*, T. Stuyver*, *J. Chem. Theory Comput.* **2025**, *21*, 8907-8917.
- What can be learned from the electrostatic environments within nitrogenase enzymes? T. Stuyver*, O. Protsenko, D. Avagliano, T. Ward*, *Chem. Eur. J.* **2025**, e202501616.

- Improving the reliability of, and confidence in, DFT functional benchmarking through active learning. J. E. Alfonso-Ramos, C. Adamo, E. Brémond*, T. Stuyver*, *J. Chem. Theory Comput.* **2025**, 21, 1752-1761.
- Graph-based deep learning models for thermodynamic property prediction: The interplay between target definition, data distribution, featurization, and model architecture. B. Deng, T. Stuyver*, *J. Chem. Inf. Model.* **2025**, 65, 649-659.
- Abiotic ribonucleoside formation in aqueous microdroplets: mechanistic exploration, acidity, and electric field effects. M. Piejko, J. E. Alfonso-Ramos, J. Moran*, T. Stuyver*, *ChemistryEurope* **2025**, e202400093.
- Combining component screening, machine learning and molecular engineering for the design of high-performance inverted perovskite solar cells. B. Zhang, H. Zeng, H. Yin, D. Zheng, Z. Wan, C. Jia, T. Stuyver*, J. Luo*, T. Pauporté*, *Energy Environ. Sci.* **2024**, 17, 5532-5541.
- Data-efficient, chemistry-aware machine learning predictions of Diels–Alder reaction outcomes. A. Keto, T. Guo, M. Underdue, T. Stuyver, C. W. Coley, X. Zhang, E. H. Krenske, O. Wiest*, *J. Am. Chem. Soc.* **2024**, 146, 16052-16061.
- TS-tools: Rapid and automated localization of transition states based on a textual reaction SMILES input. T. Stuyver*, *J. Comput. Chem.* **2024**, 45, 2308-2317.
- Repurposing quantum chemical descriptor datasets for on-the-fly generation of informative reaction representations: application to hydrogen atom transfer reactions. J. E. Alfonso-Ramos, R. M. Neeser, T. Stuyver*, *Digit. Discov.* **2024**, 3, 919-931.
- Designed local electric fields – Promising tools for enzyme engineering, S. A. Siddiqui, T. Stuyver*, S. Shaik*, K. D. Dubey*, *J. Am. Chem. Soc. Au* **2023**, 3, 3259-3269.
- Combining Molecular Modeling and Machine learning for accelerated reaction screening and discovery, N. Casetti, J. E. Alfonso-Ramos, C. W. Coley*, T. Stuyver*, *Chem. Eur. J.* **2023**, e202301957.
- 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.
- Comment on ‘physics-based representations for machine learning properties of chemical reactions’, K. A. Spiekermann, T. Stuyver, L. Pattanaik, W. H. Green*, *Mach. Learn.: Sci. Technol.* **2023**, 4, 048001.
- Machine learning-guided computational screening of new candidate reactions with high bioorthogonal click potential, T. Stuyver*, C. W. 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. W. Coley*, *Chem. Data Collect.* **2023**, 46, 101040.
- Predictive chemistry: machine learning for reaction deployment, reaction development, and reaction discovery, Z. Tu, T. Stuyver, C. W. 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. W. Coley*, *J. Chem. Phys.* **2022**, 156, 084104.
- Can the philicity of radicals be influenced by oriented external electric fields?, R. Van Lommel*, R. H. Verschuere, 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. Kenttämä, 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:

- **Chemical Compound Space Conference 2026**, March 10 – March 13, Munich (Germany); T. Stuyver, G. Chen, J. Alfonso-Ramos, “Efficient exploration of chemical reaction space via surrogate-driven chemical representations” – oral presentation
- **World Association of Theoretical and Computational Chemists (WATOC) Conference 2025**, July 22 – July 27, 2025, Oslo (Norway); T. Stuyver, “Combining chemical theory and machine learning techniques to accelerate reaction discovery” – oral presentation
- **CECAM workshop: Machine Learning Advances for Molecular and Materials Property Prediction**, July 7 – July 9, 2025, Notre Dame, Indiana (USA), T. Stuyver, “Hybrid computational chemistry – machine learning workflows for reaction screening & discovery” – oral presentation
- **11th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP)**, October 13 – October 18, 2024, Qingdao (China); T. Stuyver, Efficiently learning activation energies with ML models augmented with Valence Bond reactivity theory derived descriptors – oral presentation
- **Chemical Compound Space Conference 2024**, May 21 – May 24, 2024, Heidelberg (Germany); T. Stuyver, “Hybrid computational workflows for reaction screening & discovery” – oral presentation
- **American Chemical Society (ACS) Fall Meeting 2023**, August 13 – August 17, 2023, San Francisco (USA); T. Stuyver, “Efficiently learning reaction barriers with neural networks

augmented with descriptors derived from qualitative Valence Bond reactivity theory” – oral presentation

- **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) Conference 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

- Responsible and teacher of the course “Cheminformatics and Drug Design” in the M2 of the Science and Technology 01/09/2025 – now

for Health Master at PSL University (20 students; 18 contact hours per year)

- Responsible and teacher of the course “Theory of Chemical Reactivity” in the M2 of the Chemistry Master at PSL University (20 students; 8 contact hours per year) 01/09/2025 – now
- Teacher of the course “Data Science and AI for Chemistry” in the M2 of the Chemistry Master at PSL University (20 students; 12 contact hours per year) 01/09/2025 – now
- Track chair of the AI & Digital Health track of the Science and Technology for Health Master at PSL University 01/09/2025 – now
- Teacher of the course “Project in Cheminformatics” at ChimieParisTech – PSL University (20 students; 45 hours per year) 01/01/2023 – now
- Teacher of the exercise sessions for the first year Engineering course “Chemical Bonding” at ChimieParisTech – PSL University (20 students; 12 hours per year) 01/01/2023 – now
- 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
- Teacher 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

Organization of international conferences

- Member of the organizing committee of the QLife Winter School “AI-accelerated design and optimization of compounds for biological applications” at PSL University 09/02/2026 – 13/02/2026
- Member of the organizing committee of the CECAM workshop “Machine Learning Advances for Molecular and Materials Property Prediction” at the University of Notre Dame 07/07/2025 – 10/07/2025
- Member of the organizing committee of the one-day symposium, “Chemical Bonding in the 21st Century”, in honor of Prof. Roald Hoffmann (Brussels, Belgium) 28/05/2018

ADMINISTRATIVE DUTIES AND LEADERSHIP

- Co-coordinator of the Major Research Program of PSL University: Artificial intelligence for chemistry – ChemAI 01/01/2025 – 31/12/2029
- 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

PROFESSIONAL SKILLS

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