Thijs Stuyver – Curriculum Vitae

PERSONAL DETAILS

Citizenship: Belgian

Address: 17B Rue Pierre Honfroy, 94205 Ivry-Sur-Seine, France

Phone: +33 7 81 12 18 37

Email: thijs.stuyver@chimieparistech.psl.eu

SCIENTIFIC QUALIFICATIONS

Work Experience

Junior professor at Ecole Nationale 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 — 21/09/2015 – 07/07/2018
  magna cum laude
- Master of Science in Chemistry — 24/09/2012 – 06/07/2014
  Cluster: Molecular and macromolecular design
  summa cum laude
- Bachelor of Science in Chemistry — 22/09/2009 – 07/07/2012
  summa cum laude

DVM Humaniora Aalst — 01/09/2003 – 30/06/2009

- Sciences-Mathematics

Scholarships and Grants

- JCJC grant by Agence National de Recherche (ANR) (*research funding to hire non-permanent research staff and to buy equipment – €330.000*) — 01/10/2024
- Major Research Program of PSL University: Artificial intelligence for chemistry – ChemAI (*coordinator of a university-wide project to implement AI and automation* — 01/06/2024

across the chemistry and chemical engineering departments – €2.250.000)

- Start-up grant by Agence National de Recherche (ANR) and Centre National de Recherche Scientific (CNRS) (*research funding to hire non-permanent research staff and to buy equipment, amounting to €370.000 in total*) — 01/01/2023
- Swiss Government Excellence Scholarship awarded by the Swiss Federal Commission for Scholarships for Foreign Students (*personal research funding for 1 year – approximately €40.000*; *declined due to alternative job opportunity*) — 25/03/2021
- Marie Sklodowska-Curie Action – Individual Fellowship awarded by the European Commission (*personal research funding for 2 years – approximately €190.000*; *declined due to alternative job opportunity*) — 08/02/2021
- Research Foundation Flanders (FWO) long-term travel grant awarded (*€19.800*) — 12/11/2018
- Postdoctoral fellowship awarded by Research Foundation Flanders (*personal research funding for 3 years – approximately €180.000*) — 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 (*personal research funding for 4 years – approximately €120.000*) — 25/06/2014

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*) — 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:

- 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**, DOI: 10.1021/acs.jctc.4c01729.
- 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.
- 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. 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:

- **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

Teaching of the course "Project in Cheminformatics" at ChimieParisTech – PSL University (20 students; 45 hours per year)	01/01/2023 – now
Teaching 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
- 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 21st Century", in honor of Prof. Roald Hoffmann (Brussels, Belgium) — 28/05/2018

ADMINISTRATIVE DUTIES AND LEADERSHIP

- 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

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