Curriculum Vitae

Personal details

Title and name:	Prof. Dr. F. Matthias Bickelhaupt
Gender:	Male
Date and place of birth:	24 November 1965, Amstelveen, The Netherlands
Nationality:	German
Family status:	Married, two children
Languages:	German (native), Dutch (native), English (fluent), French, Portuguese, Spanish, Catalan (basic reading)
Website:	https://www.theochem.nl/

Publication Analysis

Publications:	**395** (+ **5** submitted/accepted/in press + **58** other publ. + **4** software)
Citations:	**29789 (WoS, core collection on 27-09-2023)**
Hirsch Index:	**73 (W**oS)
#art. 100+ cit.:	48 (WoS)
#art. 10+ cit.:	>300 (WoS)
Invited Lectures:	>200
ResearcherID:	A-3857-2009
ORCID:	0000-0003-4655-7747

Education and Career

1983 - 1988:	**Bachelor & Masters Studies** at **Vrije Universiteit Amsterdam, Netherlands (Exam: 22-06-1988)** Major in Theoretical Chemistry/Minor in Organic Chemistry/Extra in Physical Chemistry
1988 - 1993:	**Doctorate** at **University of Amsterdam, Netherlands (Defense: 17-02-1993)** Promotor: Prof. Dr. N. M. M. Nibbering, Co-Promotor: Prof. Dr. E. J. Baerends Thesis: Base-Induced Elimination Reactions - Exp. and Theor. Study on Gas-Phase Reactions
1993 - 1997:	**Postdoctoral positions** with: 1. Prof. Dr. P. von Ragué Schleyer, Universität Erlangen-Nürnberg, **Germany** 2. Prof. Dr. T. Ziegler, University of Calgary, **Canada** 3. Prof. Dr. R. Hoffmann, Cornell University, **USA** 4. Prof. Dr. E. J. Baerends, Vrije Universiteit Amsterdam, **Netherlands (NL)**
1997 - 1999:	**Assistant Professor**, Philipps-Universität Marburg, **Germany**
1999 - 2003:	**Tenured Assistant Professor**, Vrije Universiteit (VU) Amsterdam, **NL**
2003 - 2008:	**Associate Professor**, VU Amsterdam, **NL**
2009 - 2023:	**Full Professor**, VU Amsterdam, **NL**
2010 - **present**:	**Head Division of Theoretical Chemistry**, VU Amsterdam, **NL**
2012 - **present**:	**Extraordinary Professor**, Radboud University, Nijmegen, **NL**
2014 - **present**:	Fellow of the Royal Society of Chemistry (**FRSC**), **UK**
2014 - **present**:	Member **Royal Holland Society of Sciences and Humanities**, **NL**
2019 - **present**:	**Head Department of Chemistry & Pharmaceutical Sciences**, VU Amsterdam, **NL**
2020 - **present**:	**Chemistry Europe Fellow**, **EU**
2022 - **present**:	**Distinguished Visiting Professor**, University of Johannesburg, **South Africa**
2023 - **present:**	**Full Professor HL1**, VU Amsterdam, **NL**

Research Profile

In my group, we develop powerful chemical theories and methods that enable the prediction and rational design of target molecules, nanostructures, and materials, as well as new, more efficient chemical processes toward these compounds, based on quantum mechanics, *Smart AI*, and computer simulations. Topics range across the entire spectrum of the molecular sciences, from physical chemistry, via organic and inorganic chemistry, to biological and supramolecular chemistry. An essential part of these efforts is *theory-driven experimentation*, that is, the application of our theories and models in cooperation with experimental groups.

Honors, Prizes & Earning Power

1992: Shell PhD-student travel grant (Sanibel Symposium, USA)
1993-1996: Deutsche Forschungsgemeinschaft (DFG) Postdoctoral Fellowship
1997-1999: DFG Habilitation Fellowship
1998: European Union TMR Visiting Scientist, Univ. Girona, Inst. Comput. Chem.
1998-2000: Fond der Chemischen Industrie (FCI) Fellowship (1 PhD: A. Diefenbach + equipment & consumables)
2000: DAAD (German Exchange Service) Visiting Scientist, Univ. Girona, Inst. Comput. Chem.
2001-2006: Netherlands Organization for Scientific Research (NWO) Jonge Chemici award (1 PhD + equipment & consumables)
2002-2007: HPC-Europa (ca. 10 visitor grants)
2002-2008: NWO VICI award (2 PhD + 2 PD + large compute cluster + other equipment & consumables)
2004-2009: National Research School Combination - Catalysis (NRSC-C) research grant (1 PhD + 1 PD + equipment & consumables)
2004-2005: Generalitat de Catalunya (GdC) Fellowship (Host PI for 1 PD: J. Poater + equipment & consumables)
2006-2008: Marie Curie Fellowship (host PI for 1 senior PD: J. Poater + equipment & consumables)
2007: Nominated Best Teacher Faculty of Sciences
2007-2012: IRTG HRSMC-Univ. Münster funded by DFG and NWO (3 shared PhD + equipment & consumables)
2008-2012: HPC-Europa 2 (ca. 10 visitor grants)
2009-2014: IRSES grant "CANIOC" (joint proposal Girona-Spain, Amsterdam-NL, Guanajuato: network activities)
2009-2011: Ministry of Science and Education of Spain (MeC) Fellowship (host PI for 1PD: J. M. Ruíz)
2009-2015: NRSC-C research grant (1 PhD + 1 PD + equipment & consumables)
2009: Selected Teacher of the Amsterdam University College (AUC)
2009-2012: Industrial contract-research project with Wacker Chemie (1 PD + travel costs)
2010-2015: NWO Astrochemistry research grant (1 PhD + equipment & consumables)
2011: Nominated Best Teacher Faculty of Sciences
2011-2012: Basque Science Foundation Fellowship (Host PI for 1 PD: A. de Cozar + equipment & consumables)
2011-2015: NRSC-C research grant Bio-Solar Cells (1 PhD + equipment & consumables)
2012: NWO BAZIS (joint ACMM proposal: € 350,000 for parallel compute cluster)
2012: **CNPq Visiting Professor**, University of São Paulo, Ribeirão Preto, SP, Brazil (not accepted due to personal circumstances)
2012-2015: COST Action CM1005, Member (network activities)
2012-2016: COST Action CM1105, Member Management Committee (network activities)
2012-2017: NWO Graduate Program (joint HRSMC proposal: € 800,000 for 4 PhD + equipment & consumables)
2013-2019: NWO-Doctoral Grant for Teachers (1 PhD: Z. Boughlala + equipment & consumables)
2013: **European Union Visiting Professor**, Center for Advanced Studies, Warsaw University of Technology
2013: EMBO Short-Term Fellowship (host PI for 1 PD: J. Poater)
2013-2015: Marie Curie Fellowship (host PI for 1 senior PD: G. Paragi + equipment & consumables)
2013-2017: NWO Planetary and Exoplanetary Research Program (2 PD + equipment & consumables)
since 2014: Member **Koninklijke Hollandsche Maatschappij der Wetenschappen** (KHMW = Royal Holland Society of Sciences and Humanities)
2014-2015: Centro Paulo Freire hosting grant (1 visiting professor: S. E. Galembeck)
2014: Marie Curie Fellowship (host PI for 1 senior PD: G. Roos + equipment & consumables)
2014-2019: NWO Echo grant (with C. Fonseca Guerra: € 260,000: 1 PhD + 1 PD + equipment & consumables)
2014-2019: China Scholarship Council (CSC) grant (1 PhD: X. Sun)
since 2014: **Fellow of the Royal Society of Chemistry** (FRSC)
2015-2019: Shell-NWO/FOM CSER grant (€ 216,000: 1 PhD + equipment & consumables)
2016-2018: DFG Postdoctoral Fellowship (host PI for 1 PD: J. Nitsch)
2016: HRSMC hosting grant (€ 11,500: 1 visiting professor: J. Poater)
2016: China Scholarship Council (CSC) grant (1 PhD: Z. Liu)
since 2016: Member Advanced Research Center - Chemical Building Blocks Consortium (ARC CBBC)
2017-2021: China Scholarship Council (CSC) grant (1 PhD: S. Yu)
2017-2021: NWO DAN II research grant (€ 214,201: with I. Swart: 1 PhD + equipment & consumables)
2018-2019: HRSMC hosting grant (€ 1,250: 1 visiting professor: I. Fernández)
2018-2022: National Research Foundation (NRF) of South Africa (with C. Esterhuysen: 1 PhD + consumables)
2019: HRSMC hosting grant (€ 3,500: 1 visiting professor: O. Jiménez-Halla)
2019-2023: ARC-CBBC research grant (€ 400,000: Assistant Professor + PhD student)
2019-permanent: Ministry of Education and Science - Sectorplan Bèta en Techniek incl. "Van Meenen" (chair of joint Dept. Chem. & Pharm. proposal: € 1,012,000 **per year** of which € 192,000 **per year** for Comput. Chem.)
since 2020: **Chemistry Europe Fellow**
2020: **UFLA Visiting Professor**, Federal University of Lavras, Brazil (online, due to COVID-19)
2021-2023: DPI research grant (€130,000: 1 Postdoc + consumables)
2022-2026: Microsoft grant (€407,000: research project on Smart AI in quantum chemistry)
2022-present: **Distinguished Visiting Professor**, University of Johannesburg, South Africa

Teaching

1. Teaching at Philipps-Universität Marburg

1997-1998: Theoretische Chemie 1 (coordinator: G. Frenking) [in German]
1998-1999: Theoretische Anorganische Chemie (coordinator: G. Boche) [in German]
1998-1999: Chemische Bindung [in German]
1999-1999: Allgemeine und Anorganische Chemie für Biologen [in German]

2. Teaching at Vrije Universiteit Amsterdam / Bachelor courses

2000-present: Bachelor Research Projects
2000-2002: Inleiding Computer Gebruik [in Dutch]
2000-2002: Chemische Informatica [in Dutch]
2001-2002: Basiscursus Toegepaste Theoretische Chemie [in Dutch],
2001-2008: Keuzemodule Toegepaste Theoretische Chemie [in Dutch]
2001-2014: Computational (Pharmaco)Chemistry [in Dutch, #1] CC
2002-present: Bachelor Eindproject Theoretische Chemie,
2003-2005: Chemische Binding 2 [in Dutch, #2]
2004-2006: Wiskunde en Natuurwetenschappen (WNW) Practicum [in Dutch]
2005-2010: Theoretische Chemie 3 [in Dutch, #2]
2010-2012: Theoretische Chemie [in Dutch]
2011-2013: Van Atoom tot Bio-Molecuul (General Chemistry) [in Dutch]
2012-2013: Quantumchemie 2 [in Dutch, #2]
2014-present: Computationele Chemie [in Dutch, #1a] CC
2014-present: Computational Pharmaco Chemistry [in Dutch, #1b] CPC
2022-present: Quantumchemie & Modeling [in Dutch, #2] QC

3. Teaching at Vrije Universiteit Amsterdam / Master courses

2000-present: Master Research Projects (major and minor)
2000-2017: Applied Theoretical Chemistry [in English, #3]
2002-2017: Density Functional Theory for Chemists [in English, #4]
2010-2011: Highlight for Quantum Theory of Molecules & Matter [in English]
2010-2011: Highlight Statistical Theory of Complex Molecular Systems [in English]
2012-present: Molecular Computational Chemistry [in English]
2017-present: Physical Organic Chemistry [in English]
2017-2018: Chemical Bonding in Kohn-Sham DFT [in English, #4]
2017-present: Advanced Computational Chemistry [in English, #3]
2017-2018: Honors Course "How to Make an Alien" for Physics, Chemistry and Biology students [in English]
2019-present: Advanced Molecular Orbital Theory [in English, #4]

4. Teaching at Vrije Universiteit Amsterdam / Miscellaneous

2003-2014: Master Class Chemie en Misdaad ("The Chemistry of CSI" for high-school students)
2004-2009: Training for Chemistry Olympics (high-school students for national and international C.O.)

5. Teaching at Amsterdam University College (AUC) / Bachelor courses

2009-2014: Introduction to Chemistry (100 level General Chemistry; 6 ec) [in English]
2009-2018: Capstone Project (300 level research project; 18 ec) [in English]
2014-2017: Computational Chemistry and Catalysis (300 level; 6 ec) [in English]

6. Teaching at Radboud University (AUC) / Bachelor courses

2016-present: Applied Quantum Chemistry (300 level; 6 ec) [in English]

7. Teaching at various institutes / PhD courses

2013-present: Molecular Modeling [in English], HRSMC, Amsterdam, The Netherlands (3 ec) [in English]
2013: ADF Workshop, for WUT and UW, in Warsaw, Poland [in English]
2015: ADF Workshop, for USP - Ribeirão Preto, São Paulo, Brazil [in English]
2016: Contribution to ADF Workshop, for the SCM company, Amsterdam, The Netherlands [in English]
2020: Advanced Computational Chemistry, Visiting Professor at University of Lavras, Brazil [in English]

8. Other activities related to teaching

2009-2010: Member Curriculum Commission of VU and UvA universities for developing and setting up the new VU-UvA joint-degree bachelor program Chemistry in Amsterdam, which started in 2011.
2019-2021: Initiated as Head of Department, together with counterpart of UvA HIMS institute, the development of a new joint-degree bachelor program in which the "Zandlopermodel" ("hourglass model") was introduced: 4 thematic lines (Chemistry of Life + Analytics & Spectroscopy + Synthesis & sustainability + Quantum & Computing): Year 1 comprises all 4; Year 2 entails a choice of 3/4; Year 2 entails a choice of 2/4, and the bachelor project implies a choice of 1/4.

Selected External collaborations

International collaborations with the following groups:

- Prof. Dr. K. N. Houk (theoretical chemistry), UCLA, Los Angeles, CA, USA
- Prof. Dr. H. Braunschweig (inorganic chemistry)), Universität Würzburg, Germany
- Prof. Dr. T. Marder (inorganic chemistry)), Universität Würzburg, Germany
- Prof. Dr. M. Solà (theoretical chemistry), University of Girona, Catalonia, Spain
- Prof. Dr. F. Cossío (theoretical organic chemistry), University of the Basque Country, San Sebastian, Spain
- Prof. Dr. I. Fernández (theoretical organic chemistry), Universidad Complutense, Madrid, Spain
- Prof. Dr. H. F. Schaefer III (theoretical chemistry), University of Georgia, Athens, Georgia, USA
- Prof. Dr. C. Estherhuysen, University of Stellenbosch, South Africa
- Prof. Dr. Jing Xie, Beijing Institute of Technology, China
- Prof. Dr. W. D. Allen (theoretical chemistry), University of Georgia, Athens, Georgia, USA
- Prof. Dr. M. Swart (theoretical chemistry), ICREA and University of Girona, Catalonia, Spain
- Prof. Dr. G. Merino (theoretical chemistry), University of Merida, Mexico
- Prof. Dr. F. DeProft (theoretical chemistry), Vrije Universiteit Brussel, Belgium
- Prof. Dr. P. Geerlings (theoretical chemistry), Vrije Universiteit Brussel, Belgium
- Prof. Dr. L. Orian (theoretical chemistry), University of Padova, Italy
- Prof. Dr. G. Barone (theoretical chemistry), University of Palermo, Italy
- Prof. Dr. U. Radius (inorganic chemistry)), Universität Würzburg, Germany
- Dr. V. Sychrovsky (bioinorganic NMR), Academy of Sciences of the Czech Republic, Prague, Czech Republic
- Prof. Dr. T. Ramalho (theoretical chemistry), Universidade Federal de Lavras, Brazil
- Prof. Dr. J. Müller (bioinorganic chemistry), Universität Münster, Germany
- Prof. Dr. J. Mecinovic (organic chemistry), University of Southern Denmark

National collaborations with the following groups:

- Prof. Dr. F. Rutjes (organic chemistry), Radboud University, Nijmegen, The Netherlands
- Prof. Dr. A. Minnaard (organic chemistry), University of Groningenn, The Netherlands
- Prof. Dr. G. Groenenboom (theoretical chemistry), Radboud University, Nijmegen, The Netherlands
- Prof. Dr. R. V. A. Orru (organic chemistry), Maastricht University, The Netherlands
- Prof. Dr. J. Codée (organic chemistry), Leiden University, The Netherlands
- Prof. Dr. R. Sijbesma (supramolecular polymer chemistry), TU Eindhoven, The Netherlands
- Prof. Dr. H. V. J. Linnartz (laboratory astrochemistry), Leiden University, The Netherlands
- Prof. Dr. F. van Delft (organic chemistry), Wageningen University & SynAffix BV in Oss, The Netherlands
- Prof. Dr. E. Hensen (molecular catalysis), TU Eindhoven, The Netherlands
- Dr. I. Swart (STM, single molecule detection), Utrecht University, The Netherlands

Local collaborations with the following groups:

- Prof. Dr. C. Fonseca Guerra (theoretical chemistry), Vrije Universiteit Amsterdam, The Netherlands
- Dr. T. A. Hamlin (theoretical chemistry), Vrije Universiteit Amsterdam, The Netherlands
- Dr. T. A. P. Vermeeren (theoretical chemistry), Vrije Universiteit Amsterdam, The Netherlands
- Prof. Dr. E. Ruiter (organic chemistry), Vrije Universiteit Amsterdam, The Netherlands
- Dr. T. Hansen (organic chemistry), Vrije Universiteit Amsterdam, The Netherlands
- Prof. Dr. Em. K. Lammertsma (organic chemistry), Vrije Universiteit Amsterdam, The Netherlands
- Prof. Dr. E. J. Meijer (computational chemistry), University of Amsterdam, The Netherlands

Organization, Management, and other Academic Activities

- ***Member*** Royal Holland Society of Sciences and Humanities: 2014-present
- ***Member*** NWO Table Chemistry (Tafel Chemie): 2017-2023
- ***Founding Chairman***, KNCV Division CTC: 2017-2023
- ***Head*** Department of Chemistry & Pharmaceutical Sciences: 2019-present
- ***Head*** Division of Theoretical Chemistry: 2010-present
- ***Chairman of the Board*** Holland Research School of Molecular Chemistry ***(HRSMC)***: 2010-present
- ***Chairman of the Board*** Amsterdam Center for Multiscale Modeling ***(ACMM)***: 2014-present
- ***Member of the Board*** Stichting HRSMC Congresorganisatie: 2016-present
- ***Member of the Management Team*** Department of Chemistry and Pharmaceutical Sciences: 2017-present
- ***Member*** Chemie Media Centrum (Chemistry Media Center) of the KNCV (Royal Netherlands Chemical Society): 2017-present
- ***Secretary of the Board*** Division of Spectroscopy and Theory, ***Netherlands Organization for Scientific Research (NWO)***: 2008-2011
- ***Scientific Advisory Board member*** of the Institute of Computational Chemistry and Catalysis (ICCC), University of Girona: 2013-2017

- ***Scientific Advisory Board member*** of Leiden Institute of Chemistry (LIC), Leiden University: 2014-present
- ***Chair*** *Inaugural* KNCV-CTC Symposium 2019 (23. 03. 2019, National Computational &Theoretical Chem meeting, ca 120 attendants), VU Amsterdam
- ***Chair*** CBOND 2022 Amsterdam online (20-22 Sep 2020, intl. meeting via Zoom webinar, ~200 attendees), VU Amsterdam
- ***Chair*** ESOR 2021 Amsterdam online (21-23 Sep 2020, intl. meeting via Zoom webinar, ~300 attendees), VU Amsterdam
- ***Chair*** HBOND 2019 (together with C. Fonseca Guerra, 23-27 Sep 2019, intl. meeting, 113 attendees), VU Amsterdam
- ***Program Committee member*** CHAINS 2016 (Natl. Chem. Conf., ca 1500 attendants), Veldhoven: 2015-2016
- ***Editorial Advisory Board member*** of Chemistry Europe (Wiley-VCH): 2023-present
- ***Editorial Advisory Board member*** of Chemistry – A European Journal (Wiley-VCH): 2013-present
- ***International Advisory Board member*** of Chemistry – An Asian Journal (Wiley-VCH): 2013-2017
- ***Editorial Board member*** of Chemistry – An Asian Journal (Wiley-VCH): 2018-present
- ***Editorial Advisory Board member*** of ChemistryOpen (Wiley-VCH): 2011-present
- ***Editorial Advisory Board member*** of Physical Chemistry Chemical Physics (Royal Society of Chemistry): 2009-2022
- ***Editorial Advisory Board member*** of the Journal of Computational Chemistry (Wiley): 2000-present
- ***Assistant Editor*** of the Journal of Computational Chemistry (Wiley): 1998-2000
- ***Member Redactieraad (Editorial Board)*** of *Chemisch 2 Weekblad (C2W)* of the KNCV: 2021-present
- ***Chairman Program Committee***, BSc Scheikunde & MSc Chemistry for VU & UvA: 2009-2019
- ***Member Program Committee*** of the Department of Chemistry: 2002-2005
- ***Member Curriculum Commission for a joint Chemistry Bachelor*** of VU and UvA Universities: 2009-2011
- ***Taskforce member*** for the creation of a new Dept. Mol. Chem. & Life Sci. in Amsterdam, VU Amsterdam & University of Amsterdam: 2013-2017
- ***Board member*** Alumni Society Department of Chemistry & Pharmaceutical Sciences "ABC": 2014-2022
- ***Chairman*** Alumni Society Department of Chemistry & Pharmaceutical Sciences "ABC": 2022-present
- ***Coordinator VU Chemistry*** National Evaluation and Visitation of Chemistry Studies: 2012
- ***Master Coordinator*** Theoretical Chemistry: 2003-2010
- ***Member of the Public Relations committee*** of the Department of Chemistry (-2011)
- ***Member of various other commissions*** of the Department of Chemistry and the Faculty of Sciences
- ***Editor*** website Department of Chemistry & Pharmaceutical Sciences (2009-2011)
- ***Member "Top-Talent Advise Commission"*** of VU University (2007-present)
- ***Member NWO VIDI commission***: 2005-2006
- ***Member NWO TOP/ECHO commission***: 2006-2007
- ***Member NWO VENI commission***: 2007-2010
- ***Member NWO GO VENI commission***: 2010-2012
- ***Member NWO TOP/ECHO commission***: 2011-2012
- ***Member Research Foundation Flanders (FWO) Physical Chemistry commission*** (-2010)
- ***Chairman*** **Evert Jan Baerends Symposium**, Amsterdam, 2005
- ***Chairman*** **ESOR 2023**, Amsterdam, 2021-present
- ***Chairman*** **CBOND 2022**, Amsterdam, 2018-present
- ***Chairman*** **ESOR 2021**, Amsterdam, 2019-2020
- ***Scientific Committee member*** biannual **Girona Seminar**, Girona, Spain, 2006-2014
- ***International Advisory Board member*** **ICCS Comput. Chem. Workshop**, Cairns, Australia, 2014
- ***International Advisory Board member*** **Virtual Conference on Comput. Chem.**, Univ. Mauritius, 2013-2014
- ***International Advisory Board member*** **Virtual Winterschool on Comput. Chem.**, VU Brussels, 2015-2016
- ***Treasurer of Organizing Committee*** **DFT 2007 Symposium**, Amsterdam: 2007
- *Invited by the* ***Royal Swedish Academy of Sciences*** to nominate a candidate for the ***Nobel Prize in Chemistry***: 2009, 2011, 2016, 2017, 2018, 2019, 2020, 2021, 2022, 2023.
- *Invited by the* ***Royal Swedish Academy of Sciences*** to nominate a candidate for the ***Nobel Prize in Physics***: 2018, 2019, 2020, 2021, 2022, 2023.
- ***Member of Chemical Societies:*** (1) KNCV (Netherlands), (2) GDCh (Germany), (3) ACS (USA), (4) IUPAC (international), (5) WATOC (international), (6) AGTC (Germany); (7) Fellow of the RSC (UK).
- ***Referee for 19 funding agencies,*** among which: (1) Netherlands Organization of Scientific research (NWO), Netherlands, (2) European Research Council (ERC), EU, (3) Deutsche Forschungsgemeinschaft (DFG), Germany; (4) National Science Foundation (NSF), USA, (5) National Sciences and Engineering Research Council (NSERC), Canada, (6) Petroleum Research Fund (PRF), USA, (7) U.S. Department of Energy (DOE), USA, ...
- ***Referee for >100 international scientific journals,*** among which: (1) Angew. Chem.; (2) JACS; (3) Nature Chem.; (4) Nature Comm.; (5) Chem. Sci.; (6) CEJ; (7) ChemComm, ...

Participation in Academic Alliances

1. 1999-present: Department of Theoretical Chemistry, Vrije Universiteit Amsterdam, Amsterdam (home institute)
2. 1999-2014: National Research School Combination - Catalysis (NRSC-C)
3. 2000-present: Holland Research School of Molecular Chemistry (HRSMC), Amsterdam
4. 2007-2012: International Research Training Group (**IRTG**) HRSMC-University of Münster, **Germany**
5. 2008-present: Amsterdam Center for Multiscale Modeling (ACMM), Dutch node (with Lorentz Center, Leiden) of European **CECAM**
6. 2009-present: Netherlands Institute for Catalysis Research (NIOK)
7. 2010-present: Amsterdam Institute of Molecular and Life Systems (AIMMS), Vrije Universiteit Amsterdam
8. 2016-present: Member Advanced Research Center - Chemical Building Blocks Consortium (**ARC-CBBC**)
9. 2021-present: DPI

Industrial Collaborations

1. Scientific Computing & Modeling NV, Amsterdam, Netherlands: xxxx-present
2. Blum Scientific, München, Germany: completed
3. Wacker Chemie AG, München, Germany: 2009-2016
4. SynAffix, Oss, Netherlands: 2012-2015
5. Shell, Netherlands (via Shell-NWO/FOM CSER program): 2015-2020
6. AkzoNobel, Netherlands: 2017-2018
7. Nouryon, Netherlands: 2018-present
8. DSM, Netherlands: 2022-present

Ph.D. Theses Supervised

1. C. Fonseca Guerra, Structure and Bonding of DNA - Development and Application of Parallel and Order-N DFT Methods, VU University Amsterdam, The Netherlands, 22 February **2000**.
2. A. Diefenbach, Fragment-Oriented Design of Catalysts - A Theoretical Study on Bond Activation, Philipps-Universität Marburg, Germany, 20 December **2000** – cum laude.
3. G. Th. de Jong, Theoretical Studies on Catalytic Bond Activation, VU University Amsterdam, The Netherlands, 24 April **2007**.
4. S. C. A. H. Pierrefixe, Hypervalence and Aromaticity, VU University Amsterdam, The Netherlands, 2 June **2008**.
5. A. P. Bento, Elementary Chemical Reactions, VU University Amsterdam, The Netherlands, 27 October **2008**.
6. M. A. van Bochove, Nucleophilic Substitution at Phosphorus Centers, VU University Amsterdam, The Netherlands, 9 December **2008**.
7. T. van der Wijst, DNA Base Quartets and Tautomers, Universität Dortmund and Max-Planck-Institut (promotor: B. Lippert, co-promotor: F. M. Bickelhaupt), Germany, 16 October **2009**.
8. D. A. Megger, Metal-Mediated Base Pairs Containing Artificial Purine-, Phenanthroline-, and Bis(pyridine)-Derived Nucleobases, Universität Münster (promotor: J. Müller, co-promotor: F. M. Bickelhaupt), Germany, 16 October **2010** - summa cum laude.
9. W.-J. van Zeist, "Activating Bonds - Theoretical Studies of Chemical Bonds and their Catalytic Activation by Palladium", VU University Amsterdam, The Netherlands (promotor: F. M. Bickelhaupt), 15 June **2011** – cum laude.
10. K. Seubert, working title: "Metal-Mediated Base Pairs", Universität Münster (promotor: J. Müller, co-promotor: F. M. Bickelhaupt), Germany, 15 June **2012** – magna cum laude.
11. H. Kruse, "Supramolecular Quantum Chemistry: Application and Development of Methodologies for Large Systems" (promotor: S. Grimme, co-promotor: F. M. Bickelhaupt), Westfälische Wilhelms-Universität Münster, Germany, 24 August **2012**.
12. B. Zarzycki, "Element–Element Bindungsaktivierung an [Ni(*i*Pr$_2$Im)$_2$] und [(η^5-C$_5$H$_5$)Co(*i*Pr$_2$Im)]" (promotor: U. Radius, co-promotor: F. M. Bickelhaupt), Julius-Maximilians-Universität Würzburg, Germany , 21 March **2013**.
13. L. Guillaumes, "Analysis of Cooperation and Electron Delocalization in Intermolecular Hydrogen Bonds", **double degree**: University of Girona, Spain & Vrije Universiteit Amsterdam, The Netherlands (promotor: F. M. Bickelhaupt, co-promotores: C. Fonseca Guerra, S. Simon Rabasseda), 15 June **2015** + 22 June **2015**.
14. L. P. Wolters, "Chemical Bonding and Catalysis: Molecular Orbital Perspectives on Catalyst Design and Halogen Bonds", Vrije Universiteit Amsterdam, The Netherlands (promotor: F. M. Bickelhaupt), 22 March **2016** (**Dick Stufkens Prize** 2016).
15 J. P. Martinez, "Reactivity of Endohedral Fullerenes", **double degree**: Vrije Universiteit Amsterdam, 17. 05. **2017** & Universitat de Girona 19. 11. **2016** (promotores: F. M. Bickelhaupt, M. Solà).
16. Renato Orenha, "Nitrosyl Complexes", **double degree**: University of São Paulo - Ribeirão Preto, SP, Brazil, 08.

05. **2017** & Vrije Universiteit Amsterdam 05. 08. **2017** (promotores: F. M. Bickelhaupt, S. E. Galembeck).

17. M. Bortoli, "The Role of Selenium in Glutathione Peroxidase: Insights from Molecular Modeling" (Promotores: F. M. Bickelhaupt, L. Orian), **joint degree:** Vrije Universiteit Amsterdam, 17 April **2019** & University of Padova, Italy.
18. D. Césario,, "Insights from a Theoretical Approach on the Weak Intermolecular Forces: the transition from Van Der Waals to Chemical Bond " (Promotores: F. M. Bickelhaupt, F. Tarantelli; Co-Promotores: C. Fonseca Guerra, F. Nunzi), **double degree**: Vrije Universiteit Amsterdam, 7 May **2019** & University of Perugia, Italy, 26 February **2019**.
19. X. Sun, "Activating Bonds: Rational Design of Iron-Based Catalysts for Cross Coupling" (promotores: F. M. Bickelhaupt, C. Fonseca Guerra; co-promotor: T. A. Hamlin), Vrije Universiteit Amsterdam, 16 September **2019**.
20. F. Zaccaria, "G-Quadruplex: A Systematic Investigation on the Interaction of Cations with the Internal Channel site" (promotores: C. Fonseca Guerra, F. M. Bickelhaupt), Vrije Universiteit Amsterdam, 7 October **2019**.
21. J. Z. A. Laloo, "Theoretical Studies of Bimolecular Nucleophilic Substitution Reactions" (promotor: P. Ramasami; co-promotor: F. M. Bickelhaupt), University of Mauritius, Mauritius, 8 October **2019**.
22. S. C. C. van der Lubbe, "The Nature of Hydrogen Bonds" (promotores: C. Fonseca Guerra, F. M. Bickelhaupt), Vrije Universiteit Amsterdam, 16 October **2019**
23. A. K. Narsaria, "Design of Organic Solar Cells" (promotores: F. M. Bickelhaupt, K. Lammertsma; co-promotor: A. W. Ehlers, C. Fonseca Guerra), Vrije Universiteit Amsterdam, 18 June **2020**.
24. Z. Boughlala, "Cation Affinities throughout the Periodic Table" (promotores: F. M. Bickelhaupt, C. Fonseca Guerra), Vrije Universiteit Amsterdam, 15 October **2020**.
25. M. Dalla Tiezza, "A Quantitative Kohn–Sham Approach to Elementary Redox Reactions in Artificial, Bio-Inspired and Biological Catalysis" (promotores: L. Orian, F. M. Bickelhaupt), **joint degree** (with Univ. Padova, Italy): Vrije Universiteit Amsterdam, 20 September **2021**.
26. Lucas Azevedo, "Intermolecular Covalent Interactions - A Quantitative Molecular Orbital Perspective" (promotores: F. M. Bickelhaupt, T. Ramalho; co-promotor: T. A. Hamlin), **double degree** (with UFLA, Brazil) Vrije Universiteit Amsterdam, 2 November **2021**.
27. S. Yu, Cycloaddition Reactions - Design Principles from Quantum Chemical Analyses (promotor: F. M. Bickelhaupt; co-promotor: T. A. Hamlin), Vrije Universiteit Amsterdam, 14 December **2021**.
28. P. Vermeeren, "(Astro)Chemistry - From Molecules to Reactions" (promotor F. M. Bickelhaupt; co-promotor: T. A. Hamlin), Vrije Universiteit Amsterdam, 15 February **2022** – **cum laude**
29. E. Blokker, "##>Tuning Initiators for the Formation of Polymer Materials<##" (promotor: F. M. Bickelhaupt; co-promotores: T. A. Hamlin, J. M. van der Schuur [Nouryon]), Vrije Universiteit Amsterdam, ***planned for*** **2023**.
30. B. Moloto, "##>Bond Activation by Gold(I) Dimer Complexes<##" (promotores: C. Esterhuysen, F. M. Bickelhaupt), double degree: Vrije Universiteit Amsterdam & Universiteit Stellenbosch, ***planned for*** **2023**.
31. C. Nieuwland, "##>DNA Replication<##" (promotores: F. M. Bickelhaupt, C. Fonseca Guerra; co-promotor: T. A. Hamlin), Vrije Universiteit Amsterdam, ***planned for*** **2024**.
32. S. Beutick "##> Reactivity in Organic and Biological Chemistry<##" (promotores: F. M. Bickelhaupt, L. Prian; co-promotor: T. A. Hamlin), **joint degree** (with Univ. Padova, Italy): Vrije Universiteit Amsterdam, ***planned for*** **2024**.
33. E. Tiekink, "##>Theory-Driven Experimentation<##" (promotor: F. M. Bickelhaupt; co-promotor: T. A. Hamlin), Vrije Universiteit Amsterdam, ***planned for*** **2025**.
34. Y. Hordijk, "##>Smart AI<##" (promotor: F. M. Bickelhaupt; co-promotor: T. A. Hamlin), Vrije Universiteit Amsterdam, ***planned for*** **2026**.

Selected Publications

- L. de Azevedo Santos, T. C. Ramalho, T. A. Hamlin, F. M. Bickelhaupt —— "Intermolecular Covalent Interactions: Nature and Directionality" —— *Chem. Eur. J.* **2022**, *28*, online.
- S. Yu, E. H. Tiekink, P. Vermeeren, F. M. Bickelhaupt, T. A. Hamlin —— "How Bases Catalyze Diels-Alder Reactions" —— *Chem. Eur. J.* **2022**, *28*, online.
- T. Hansen, P. Vermeeren, F. M. Bickelhaupt, T. A. Hamlin —— "Stability of Alkyl Carbocations" —— *Chem. Comm.* **2022**, *58*, 12050-12053 (Cover). Highlighted in C2W. Highlighted in C2W International. Highlighted in *Chemistry World*.
- P. Vermeeren, F. M. Bickelhaupt —— "The Abnormally Long and Weak Methylidyne C–H Bond" —— *Nat. Sci.* **2022**, *2*, e20220039.
- E. Blokker, W.-J. van Zeist, X. Sun, J. Poater, J. M. van der Schuur, T. A. Hamlin, F. M. Bickelhaupt —— "Methyl Substitution Destabilizes Alkyl Radicals" —— *Angew. Chem.* **2022**, *134*, e202207477/1-6; *Angew. Chem. Int. Ed.* **2022**, *61*, e202207477/1-6. Highlighted in C2W. Highlighted by ARC CBBC.

- P. Vermeeren, M. Dalla Tiezza, M. E. Wolf, M. E. Lahm, W. D. Allen, H. F. Schaefer III, T. A. Hamlin, F. M. Bickelhaupt —— "**Pericyclic Reaction Benchmarks**: Hierarchical Computations Targeting **CCSDT(Q)/CBS** and Analysis of DFT Performance" —— *Phys. Chem. Chem. Phys.* **2022**, *24*, 18028-18042 (Themed Collection 2022 PCCP HOT Articles).
- C. Nieuwland, T. A. Hamlin, C. Fonseca Guerra, G. Barone, F. M. Bickelhaupt —— "B-DNA Structure and Stability: The Role of Nucleotide Composition and Order" —— *ChemistryOpen* **2022**, *11*, e202100231/1-14 (Quantum Bioinorganic Chemistry (QBIC) special collection, Cover & Cover Profile).
- T. Hansen, X. Sun, M. Dalla Tiezza, W.-J. van Zeist, J. Poater, T. A. Hamlin, F. M. Bickelhaupt —— "C(sp^n)–X (n = 1–3) Bond Activation by Palladium" —— *Chem. Eur. J.* **2022**, *28*, e202103953/1-7.
- T. Hansen, J. C. Roozee, F. M. Bickelhaupt, T. A. Hamlin —— "How Solvation Influences the S_N2 versus E2 Competition" —— *J. Org. Chem.* **2022**, *87*, 1805-1813.
- J. J. A. G. Kamps, R. Belle, J. Poater, K. Kumar, B. J. G. E. Pieters, T. Brown, T. D. W. Claridge, R. S. Paton, F. M. Bickelhaupt, A. Kawamura, C. J. Schofield, J. Mecinovic —— "Reading and Erasing of the Phosphonium Analogue of Trimethyllysine by Epigenetic Proteins" —— *Commun. Chem.* **2022**, *5*, 27/1-11.
- E. Blokker, X. Sun, J. Poater, J. M. van der Schuur, T. A. Hamlin, F. M. Bickelhaupt —— "The Chemical Bond: When Atom Size Instead of Electronegativity Difference Determines Trends in Bond Strength" —— *Chem. Eur. J.* **2021**, *27*, 15616-15622 (Cover, Communication). Highlighted in ChemistryViews, 27 October 2021 Highlighted in *C2W*, 12 November **2021**. Highlighted in *C2W International*, *(issue 5)* **2021**. Highlighted in *Chemistry World*, *16 November* **2021**. Highlighted in *Nature Briefing*, 17 November **2021**.
- P. Vermeeren, W.-J. van Zeist, T. A. Hamlin, C. Fonseca Guerra, F. M. Bickelhaupt —— "Not Carbon s–p Hybridization, but Coordination Number Determines C–H and C–C Bond Length" —— *Chem. Eur. J.* 2021, *27*, 7074-7079 (Cover). See also Feature by D. Linzel in *C2W International* **2021**, 3.
- Hansen, P. Vermeeren, F. M. Bickelhaupt, T. A. Hamlin —— "Origin of the alpha-Effect in S_N2 Reactions" —— *Angew. Chem.* **2021**, *133*, 21008-21016; *Angew. Chem. Int. Ed.* **2021**, *60*, 20840-20848 (Cover).
- P. Vermeeren, T. A. Hamlin, F. M. Bickelhaupt —— "Chemical Reactivity from an Activation Strain Perspective" —— *Chem. Commun.* **2021**, *57*, 5880-5896 (Feature Article, Cover).
- T. A. Hamlin, F. M. Bickelhaupt, I. Fernandez —— "The Pauli-Repulsion Lowering Concept in Catalysis" —— *Acc. Chem. Res.* **2021**, *54*, 1972-1981 (Cover).
- P. Vermeeren, M. Dalla Tiezza, M. van Dongen, I. Fernandez, F. M. Bickelhaupt, T. A. Hamlin —— "Lewis Acid-Catalyzed Diels-Alder Reactions: Reactivity Trends Across the Periodic Table" —— *Chem. Eur. J.* **2021**, *27*, 10610-10620.
- D. Rodrigues Silva, L. de Azevedo Santos, T. A. Hamlin, C. Fonseca Guerra, M. P. Freitas, F. M. Bickelhaupt —— "The *Gauche* Effect in XCH_2CH_2X Revisited" —— *ChemPhysChem* **2021**, *22*, 641-648.
- P. Vermeeren, M. T. Doppert, F. M. Bickelhaupt, T. A. Hamlin —— "How Metallylene Catalysts Activate Small Molecules" —— *Chem. Sci.* **2021**, *12*, 4526-4535.
- P. Vermeeren, T. A. Hamlin, F. M. Bickelhaupt, I. Fernandez —— "Bifunctional Hydrogen Bond Donor-Catalyzed Diels-Alder Reactions: Origin of Selectivity and Rate Enhancement" —— *Chem. Eur. J.* 2021, *27*, 5180-5190 (Cover, Hot Paper).
- S. Yu, P. Vermeeren, T. A. Hamlin, F. M. Bickelhaupt —— "How Oriented External Electric FieldsModulate Reactivity" —— *Chem. Eur. J.* **2021**, *27*, 5683-5693 (Cover).
- P. Vermeeren, T. Hansen, P. Jansen, M. Swart, T. A. Hamlin, F. M. Bickelhaupt —— "A Unified Framework for Understanding Nucleophilicity and Protophilicity in the S_N2/E2 Competition" —— *Chem. Eur. J.* **2020**, *26*, 15538-15548 (Cover, issue #1000).
- K. Oberdorf, A. Hanft, J. Ramler, I. Krummenacher, F. M. Bickelhaupt, J. Poater, C. Lichtenberg —— "Bismuth Amides (Re-)Investigated: Mediators of Facile and Highly Selective Pn–Pn Radical Coupling Reactions (Pn = N, P, As)" —— *Angew. Chem.* **2021**, *133*; *Angew. Chem. Int. Ed.* **2021**, *60*, online.
- S. C. C. van der Lubbe, P. Vermeeren, C. Fonseca Guerra, F. M. Bickelhaupt—— "The Nature of Nonclassical Carbonyl Ligands Explained by Kohn-Sham Molecular Orbital Theory" —— *Chem. Eur. J.* **2020**, *26*, 15690-15699 (issue #1000).
- P. Vermeeren, T. A. Hamlin, I. Fernandez, F. M. Bickelhaupt —— "Origin of Rate Enhancement and Asynchronicity in Iminium Catalyzed Diels-Alder Reactions" —— *Chem. Sci.* **2020**, *11*, 8105-8112 (Cover).
- B. J. G. E. Pieters, M. H. M. Wuts, J. Poater, K. Kumar, P. B. White, J. J. A. G. Kamps, W. Sherman, G. J. M. Pruijn, R. S. Paton, T. Beuming, F. M. Bickelhaupt, J. Mecinovic —— "Mechanism of Biomolecular Recognition of Trimethyllysine by the Fluorinated Aromatic Cage of Epigenetic Reader Proteins" —— *Commun. Chem.* **2020**, 3, 69/1-12.
- J. Jian, J. Poater, P. B. White, C. J. McKenzie, F. M. Bickelhaupt, J. Mecinovic —— "Probing Halogen–π versus

CH–π Interactions in Molecular Balance" —— *Org. Lett.* **2020**, *22*, 7870-7873.

- A. Narsaria, F. Rauch, J. Krebs, P. Endres, A. Friedrich, I. Krummenacher, H. Braunschweig, M. Finze, J. Nitsch, F. M. Bickelhaupt, T. B. Marder —— "Computationally Guided Molecular Design to Minimize the LE/CT Gap in D-π-A Fluorinated Triarylboranes for Efficient TADF via D and π-Bridge Tuning" —— *Adv. Funct. Mater.* **2020**, *30*, 2002064/1-15.
- P. Vermeeren, T. A. Hamlin, I. Fernandez, F. M. Bickelhaupt —— "How Lewis Acids CatalyzeDiels-Alder Reactions" —— *Angew. Chem.* **2020**, *132*, 6260-6265; *Angew. Chem. Int. Ed.* **2020**, *59*, 6201-6206.
- P. Vermeeren, S. C. C. van der Lubbe, C. Fonseca Guerra, F. M. Bickelhaupt, T. A. Hamlin —— "Understanding Chemical Reactivity Using the Activation Strain Model" —— *Nature Protoc.* **2020**, *15*, 649-667.
- A. K. Narsaria, J. Poater, C. Fonseca Guerra, A. W. Ehlers, T. A. Hamlin, K. Lammertsma, F. M. Bickelhaupt —— "Distortion-Controlled Red-Shift of Organic Dye Molecules" —— *Chem. Eur. J.* **2020**, *26*, 2080-2093.
- T. Bettens, M. Alonso, F. De Proft, T. A. Hamlin, F. M. Bickelhaupt —— "Ambident Nucleophilic Substitution: Understanding Non-HSAB Behavior through Activation Strain and Conceptual DFT Analyses" —— *Chem. Eur. J.* **2020**, *26*, 3884-3893.
- T. A. Hamlin, I. Fernandez, F. M. Bickelhaupt —— "How Dihalogens Catalyze Michael Addition Reactions" —— *Angew. Chem.* **2019**, *131*, 9015-9020; *Angew. Chem. Int. Ed.* **2019**, *58*, 8922-8926 (Highlighted in Chemistry World: "Quantum mechanical mechanism behind 100-year-old textbook reaction revealed").
- A. K. Narsaria, T. A. Hamlin, K. Lammertsma, F. M. Bickelhaupt —— "Dual Activation of Aromatic Diels-Alder Reactions" —— *Chem. Eur. J.* **2019**, *25*, 9902-9912 (Cover & Hot Paper).
- T. A. Hamlin, B. J. Levandowski, A. K. Narsaria, K. N. Houk, F. M. Bickelhaupt —— "Structural Distortion of Cycloalkynes Influences Cycloaddition Rates both by Strain and Interaction Energies" —— *Chem. Eur. J.* **2019**, *25*, 6342-6348 (Cover).
- X. Sun, M. V. J. Rocha, T. A. Hamlin, J. Poater, F. M. Bickelhaupt —— "Understanding the Differences Between Iron and Palladium in Cross-Coupling Reactions" —— *Phys. Chem. Chem. Phys.* **2019**, *21*, 9651-9664 (Cover).
- J. Ramler, J. Poater, F. Hirsch, B. Ritschel, I. Fischer, F. M. Bickelhaupt, C. Lichtenberg —— "Facile Insertion of Carbon Monoxide into a Bismuth–Nitrogen Bond" —— *Chem. Sci.* **2019**, *10*, 4169-4176.
- Z. Boughlala, C. Fonseca Guerra, F. M. Bickelhaupt —— "Cation Affinities throughout The Periodic Table" —— In: *Advances in Inorganic Chemistry*; R. van Eldik, R. Puchta, Eds.; Academic Press: San Diego, **2019**, Vol. 73, Chapter 6, pp. 123-158 (Thematic volume devoted to 'Computational Chemistry'). [free access till 10 April 2019]
- P. Vermeeren, X. Sun, F. M. Bickelhaupt —— "Arylic C–X Bond Activation by Palladium Catalysts: Activation-Strain Analyses of Reactivity Trends" —— *Scientific Reports* **2018**, *8*, 10729/1-10.
- M. A. van Bochove, G. Roos, C. Fonseca Guerra, T. A. Hamlin, F. M. Bickelhaupt —— "How Mg^{2+} Ions Lower the S_N2@P Barrier in Enzymatic Triphosphate Hydrolysis" —— *Chem. Commun.* **2018**, *54*, 3448-3451 (Cover).
- T. A. Hamlin, B. van Beek, L. P. Wolters, F. M. Bickelhaupt —— "Nucleophilic Substitution in Solution: Activation Strain Analysis of Weak and Strong Solvent Effects" —— *Chem. Eur. J.* **2018**, *24*, 5927-5938.
- B. Ritschel, J. Poater, H. Dengel, F. M. Bickelhaupt, C. Lichtenberg —— "Double CH Activation of a Masked Cationic Bismuth Amide" —— *Angew. Chem.* **2018**, *130*, 3887-3891; *Angew. Chem. Int. Ed.* **2018**, *57*, 3825-3829.
- F. M. Bickelhaupt, K. N. Houk —— "Analyzing Reaction Rates with the Distortion/Interaction-Activation Strain Model" —— *Angew. Chem.* **2017**, *129*, 10204-10221 (Frontispiece & Cover); *Angew. Chem. Int. Ed.* **2017**, *56*, 10070-10086 (Frontispiece & Cover).
- M. G. Goesten, R. Hoffmann, F. M. Bickelhaupt, E. J. M. Hensen —— "8-Coordinate Fluoride in a Silicate Double-4-Ring" —— *Proc. Nat. Acad. Sci.* **2017**, *114*, 828-833 (highlighted in: *Science* **2017**, *355*, 592-593).
- M. G. Goesten, M. Rahm, F. M. Bickelhaupt, E. J. M. Hensen —— "Cesium's Off-the-map Valence Orbital" —— *Angew. Chem.* **2017**, *129*, 9904-9908; *Angew. Chem. Int. Ed.* **2017**, *56*, 9772-9776.
- E. Vengut-Climent, I. Gomez-Pinto, R. Lucas, P. Penalver, A. Avino, C. Fonseca Guerra, F. M. Bickelhaupt, R. Eritja, C. Gonzalez, J. C. Morales —— "Glucose-Nucleobase Pseudo Base Pairs: Biomolecular Interactions within DNA" —— *Angew. Chem.* **2016**, *128*, 8785-8789; *Angew. Chem. Int. Ed.* **2016**, *55*, 8643-8647.
- M. G. Goesten, C. Fonseca Guerra, F. Kapteijn, J. Gascon, F. M. Bickelhaupt —— "Six-coordinate Group-13 Complexes: Role of d Orbitals and Electron-Rich Multi-center Bonding" —— *Angew. Chem. Int. Ed.* **2015**, *54*, 12034-12038 (VIP + Cover).
- J. J. A. G. Kamps, J. Huang, J. Poater, C. Xu, B. J. G. E. Pieters, A. Dong, J. Min, W. Sherman, T. Beuming, F. M. Bickelhaupt, H. Li, J. Mecinovic —— "Chemical Basis for the Recognition of Trimethyllysine by Epigenetic

Reader Proteins" —— *Nature Commun.* **2015**, *6*, 8911/1-12.

- L. P. Wolters, R. Koekkoek, F. M. Bickelhaupt —— "Role of Steric Attraction and Bite-Angle Flexibility in Metal-Mediated C–H Bond Activation" —— *ACS Catalysis* **2015**, *5*, 5766-5775.
- F. Hering, J. Nitsch, U. Paul, A. Steffen, F. M. Bickelhaupt, U. Radius —— "Bite-Angle Bending as a Key for Understanding Group-10 Metal Reactivity of d^{10}-[$M(NHC)_2$] Complexes with Sterically Modest NHC Ligands" —— *Chem. Sci.* **2015**, *6*, 1426-1432.
- L. P. Wolters, F. M. Bickelhaupt —— "The Activation Strain Model & Molecular Orbital Theory" —— *WIRES Comput. Mol. Sci.* **2015**, *5*, 324-343.
- J. Dommerholt, O. van Rooijen, A. Borrmann, C. Fonseca Guerra, F. M. Bickelhaupt, F. L. van Delft —— "Highly Accelerated Inverse Electron-Demand Cycloaddition of Electron-Deficient Azides with Aliphatic Cyclooctynes" —— *Nature Commun.* **2014**, *5*, 5378/1-7.
- L. P. Wolters, W. J. van Zeist, F. M. Bickelhaupt —— "d Regime, s Regime and Intrinsic Bite-Angle Flexibility: New Concepts for Designing d^{10}-ML_n Catalysts" —— *Chem. Eur. J.* **2014**, *20*, 11370-11381 (cover).
- I. Fernandez, F. M. Bickelhaupt —— "Activation Strain Model and Molecular Orbital Theory: Understanding and Designing Chemical Reactions of Chemical Reactivity" —— *Chem. Soc. Rev.* **2014**, *43*, 4953-4967.
- H. Zijlstra, T. Leon, A. de Cozar, C. Fonseca Guerra, D. Byrom, A. Riera, X. Verdaguer, F. M. Bickelhaupt —— "Stereodivergent S_N2@P Reactions of Borane Oxazaphospholidines: Experimental and Theoretical Studies" —— *J. Am. Chem. Soc.* **2013**, *135*, 4483-4491.
- B. M. Day, T. Pugh, D. Hendriks, C. Fonseca Guerra, D. J. Evans, F. M. Bickelhaupt, R. A. Layfield —— "Normal-to-Abnormal Rearrangement and NHC Activation in Three-Coordinate Iron(II) Carbene Complexes" —— *J. Am. Chem. Soc.* **2013**, *135*, 13338-13341.
- J. Poater, M. Swart, C. Fonseca Guerra, F. M. Bickelhaupt —— "Selectivity in DNA Replication. Interplay of Steric Shape, Hydrogen Bonds, π-Stacking and Solvent Effects" —— *Chem. Commun.* **2011**, *47*, 7326-7328.
- J. Wassenaar, E. Jansen, W.-J. van Zeist, F. M. Bickelhaupt, M. A. Siegler, A. L. Spek, J. N. H. Reek —— "Catalyst Selection based on Intermediate Stability measured by Mass Spectrometry" —— *Nature Chem.* **2010**, *2*, 417-421 (News of the Week in *C&EN* 2010, April 5, p. 7).
- S. C. A. H. Pierrefixe, C. Fonseca Guerra, B. van Stralen, J. N. P. van Stralen, F. M. Bickelhaupt —— "Hypervalent Carbon Atom. "Freezing" the S_N2 Transition State" —— *Angew. Chem.* **2009**, *121*, 6591-6593; *Angew. Chem. Int. Ed.* **2009**, *48*, 6469-6471.
- T. van der Wijst, C. Fonseca Guerra, M. Swart, F. M. Bickelhaupt, B. Lippert —— "A Ditopic Ion-Pair Receptor Based on Stacked Nucleobase Quartets" —— *Angew. Chem.* **2009**, *121*, 3335-3337; *Angew. Chem. Int. Ed.* **2009**, *48*, 3285-3287.
- M. Swart, F. M. Bickelhaupt —— "QUILD: QUantum-regions Interconnected by Local Descriptions" —— *J. Comput. Chem.* **2008**, *29*, 724-734.
- S. C. A. H. Pierrefixe, F. M. Bickelhaupt —— "Aromaticity. Molecular Orbital Picture of an Intuitive Concept" —— *Chem. Eur. J.* **2007**, *13*, 6321-6328.
- M. A. van Bochove, M. Swart, F. M. Bickelhaupt —— "Nucleophilic Substitution at Phosphorus (SN2@P): Disappearance and Reappearance of Reaction Barriers" —— *J. Am. Chem. Soc.* 2006, *128*, 10738-10744.
- F. M. Bickelhaupt, H. L. Hermann, G. Boche —— "α-Stabilization of Carbanions: Fluorine Stabilizes more Effectively than the Heavier Halogens" —— *Angew. Chem.* **2006**, *118*, 838-841; *Angew. Chem. Int. Ed.* **2006**, *45*, 823-826.
- M. Swart, C. Fonseca Guerra, F. M. Bickelhaupt —— "Hydrogen Bonds of RNA are Stronger than Those of DNA, But NMR Monitors Only Presence of Methyl Substituent in Uracil/Thymine" —— *J. Am. Chem. Soc.* **2004**, *126*, 16718-16719 (*communication*).
- C. Fonseca Guerra, J.-W. Handgraaf, E. J. Baerends, F. M. Bickelhaupt —— "Voronoi Deformation Density (VDD) charges. Assessment of the Mulliken, Bader, Hirshfeld, Weinhold and VDD methods for Charge Analysis" —— *J. Comput. Chem.* **2004**, *25*, 189-210.
- C. Fonseca Guerra, F. M. Bickelhaupt —— "Orbital Interactions in Strong and Weak Hydrogen Bonds Essential for DNA Replication" —— *Angew. Chem.* **2002**, *114*, 2194-2197; *Angew. Chem. Int. Ed.* **2002**, *41*, 2092-2095.
- F. M. Bickelhaupt, R. L. DeKock, E. J. Baerends —— "The Short N-F Bond in N2F+ and How Pauli Repulsion Influences Bond Lengths. Theoretical Study of N_2X^+, NF_3X^+ and NH_3X^+ (X = F, H)" —— *J. Am. Chem. Soc.* **2002**, *124*, 1500-1505.
- G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders, T. Ziegler —— "Chemistry with ADF" —— *J. Comput. Chem.* **2001**, *22*, 931-967.

- F. M. Bickelhaupt, E. J. Baerends —— "Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry" —— In: *Rev. Comput. Chem.*; K. B. Lipkowitz and D. B. Boyd, Eds.; Wiley-VCH: New York, **2000**, *Vol. 15*, pp. 1-86.
- C. Fonseca Guerra, F. M. Bickelhaupt —— "Charge Transfer and Environment Effects Responsible for Characteristics of DNA Base Pairing" —— *Angew. Chem.* **1999**, *111*, 3120-3122. *Angew. Chem. Int. Ed.* **1999**, *38*, 2942-2945.
- F. M. Bickelhaupt —— "Understanding Reactivity with Kohn-Sham MO Theory. The E2–S_N2 Mechanistic Spectrum and other Concepts" —— *J. Comput. Chem.* **1999**, *20*, 114-128.

National Chemistry Research Evaluation

The Theoretical Chemistry group has been rated **excellent** and awarded the maximum score (**5 - 5 - 5 - 5**) by an international Chemistry Review Committee in 2010, which has assessed chemistry research at universities across the Netherlands. The Committee describes the Theoretical Chemistry group at Vrije Universiteit Amsterdam as: "A top leading research group both nationally and worldwide, with an outstanding reputation for its innovative and exceptionally high-quality research".