# Curriculum Vitae


## Marcel Swart

**Professor Dr. FYAE FRSC MAE**


6 May 2026

### 1 Personal details


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### 2 Appointments

| | |
|---|---|
| *xx/2026 – present* | *Part-time Honorary Full Professor at Zernike Institute, University of Groningen* |
| 12/2024 – present | Part-time Full Professor at IQCC Institute, University of Girona<br>10% dedication |
| 09/2009 – present | ICREA Professor at IQCC Institute, University of Girona<br>90% dedication since 12/2024, 100% dedication before |
| 07/2015 – 06/2023 | Director of IQCC Institute, University of Girona |
| 06/2006 – 09/2009 | ICREA Júnior Fellow at IQCC Institute, University of Girona |
| 05/2004 – 05/2006 | VICI Postdoctoral fellow Prof. Bickelhaupt, VU University Amsterdam |
| 05/2002 – 05/2004 | Chemistry of Complex Molecules Postdoctoral fellow Prof. Lammertsma, Dr. Ehlers, VU University Amsterdam |

### 3 Education

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|---|---|
| 03/1998 – 09/2002 | PhD Theoretical Chemistry, University of Groningen (Netherlands)<br>“Density Functional Theory Applied to Copper Proteins”<br>Supervisors: Prof HJC Berendsen, Prof GW Canters, Prof JG Snijders<br>Reading committee: Prof BW Dijkstra, Prof K Lammertsma, Prof AE Mark |
| 08/1996 | MSc Organic Chemistry, University of Groningen (Netherlands) |

### 4 Honours and awards

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|---|---|
| 06/2025 | Horizon Award by Royal Society of Chemistry |
| 06/2019 | Elected member of Academia Europaea |
| 09/2017 | Special award in honour of continuous support for advancing chemical sciences in Serbia (120 years anniversary of Serbian Chemical Society), as first and only foreigner |
| 06/2017 | Award for Best Paper in 2016 at the University of Belgrade (Serbia) with Maja Gruden |
| 11/2015 | Elected Fellow of the Royal Society of Chemistry |
| 10/2014 | Elected Fellow of the Young Academy of Europe |
| 06/2012 | Silver Jubilee Prize from Molecular Graphics and Modelling Society |
| 06/2010 | Premi Extraordinari for best PhD thesis under my supervision: Dr. Sílvia Osuna |
| 06/2009 | Premi Extraordinari for best PhD thesis under my supervision: Dr. Mireia Güell |
| 09/2005 | Young Scientist Excellent Award, *International Conference of Computational Methods in Science and Engineering* (ICCMSE), Loutraki, Greece |

## 5 List of selected invited presentations

Since 2001 I have presented more than 40 invited talks, more than 25 contributed talks and over 40 posters at national and international conferences

(selected Invited * / Keynote ** / Plenary *** talks)

12/2026 * 12th Asian Bioinorganic Chemistry Conference (AsBIC), Jaipur (IN)
06/2026 ** 46th International Conference on Coordination Chemistry (ICCC), Odense (DK)
09/2025 ** 7th EuChemS Inorganic Chemistry Conference (EICC7), Belgrade (RS)
07/2025 * International Conference on Biological Inorganic Chemistry (ICBIC), Long Beach (USA)
08/2024 * 20th International conference on DFT (DFT2024), Paris (FR)
08/2024 ** 17th European Biological Inorganic Chemistry (EuroBic) conference, Münster (DE)
07/2024 * 45th International Conference on Coordination Chemistry (ICCC), Ft. Collins (USA)
06/2024 * Contemporary Coordination Chemistry Copenhagen (C4), Copenhagen (DK)
06/2024 * Chemistry@Sete: Challenges in Computational Homogeneous Catalysis, Sète (FR)
09/2023 * 6th EuChemS Inorganic Chemistry Conference (EICC6), Vienna (AT)
08/2023 * 6th Quantum Bio-Inorganic Chemistry meeting (QBIC-VI), Warsaw (PL)
07/2023 * Larry Que Fest (40 Years of Fun with Iron Chemistry), Minnesota (USA)
08/2022 * 44th International Conference on Coordination Chemistry (ICCC), Rimini (IT)
01/2020 * Metals in Biology Gordon Research Conference (GRC-2020, Late Breaking talk), Ventura (CA, USA)
12/2019 * 35th Winter School in Theoretical Chemistry 2019: Inorganic Chemistry, Helsinki (FI)
08/2019 * 19th International Conference on Biological Inorganic Chemistry (ICBIC), Interlaken (CH)
05/2019 * 7th international conference on Biological Inorganic Chemistry (CANBIC7), Parry Sound (CAN)
11/2018 * Annual Joint Meeting Academia Euopaea and Young Academy of Europe (Building Bridges), Barcelona (ES)
09/2018 * Quantum Bio-Inorganic Chemistry meeting (QBIC-IV), Bath (UK)
07/2018 * 11th Congress on Electronic Structure and Principle (ESPA2018), Toledo (ES)
07/2018 * International Conference on Porphyrins and Phthalocyanins (ICPP10), Munich (DE)
06/2018 * 16th International Conference on Quantum Chemistry (ICQC), Menton (FR)
08/2017 * Congress of World Association of Theoretical/Computational Chemists (WATOC), Munich (DE)
06/2017 ** FemEx 2017. Promoting female excellence in theoretical chemistry, Putten (NL)
03/2017 ** The Netherlands Catalysis and Chemistry Conference (N3C), Noordwijkerhout (NL)
03/2017 *** PAC Symposium, Utrecht (NL)
10/2016 * Joint-Symposium on Theoretical and Computational Science of Complex Systems, Kyoto (JP)
09/2016 *** VII Current Trends in Theoretical Chemistry, Kraków (PL)
06/2016 *** 53rd Annual meeting of Serbian Chemical Society, Kragujevac (RS)

Furthermore, I have given more than 20 invited talks at institutions and research labs (selection):

Univ. Brussels (2024) – Hylleraas Center, Univ. Oslo (2023) – SDU Odense (2023) – IIT Roorkee (2021online) – LMU Munich (2021online) – Univ. Oxford (2020online) – Univ. Sheffield (2020online) – Univ. Bayreuth (2020) – Univ. Helsinki (2019) – Univ. Leuven (2019) – SD Univ. Odense (2019) – UvA Amsterdam (2018) – Max Planck Institute Stuttgart (2018) – Univ. Padova (2018) – Ewha Univ. Korea (2016) – KTH Stockholm (2016) – Univ. Groningen (2015) – Univ. Uppsala (2013) – Univ. Dublin (2013) – Techn. Univ. Berlin (2013) – Houk group, UCLA (2012) – Univ. Belgrade (2012) – Univ. Tromsø (2011)

## 6 List of selected public engagement of science and science policy activities

05/2023 Pint of Science, Girona
02/2022 COST Academy event Sustainability of COST Actions, COST Association, (online)
02/2021 QBtopIC discussion panel (session leader), QBIC Society, (online)
02/2021 COST Action Chairs Forum, COST Association, (online)
10/2019 Discussion meeting Young Science and Engineering Network, Groningen (NL)
05/2019 Promotor Doctor Honoris Causa Prof. EJ Baerends, Girona (ES)
09/2018 Validation workshop for 'Study on career impacts of ERC funding', Brussels (BE)
04/2018 Annual meeting EuroDoc, Tampere (FI)
04/2018 Panel member Foster Open Science (H2020), Barcelona (ES)
01/2018 Panel member ALLEA Workshop "Ethical aspects of Open Access", Brussels (BE)
*10/2017 Panel SAPEA Workshop, Talinn (EE) (cancelled, family circumstances)*
09/2017 Panel member SAPEA Workshop, Madrid (ES)
09/2017 Panel member AE/ALLEA/YAE meeting, Budapest (HU)
04/2015 EC Workshop "A vision on Open Science in 2030", Brussels (BE)
05/2012 TEDxUdG, "I'm a Chemist….."

## 7 Research funding

I have secured ca. 10m EUR for science, outreach and equipment from Spanish and Catalan Governments, the European Union (FP7, H2020) and Industry. Currently active are:

- MCIU/AEI R&D Project "QC4All", 137.500€ + FPI (PI), 2024-2027
- Postdoc Fellowship: JdC M. Ansari, 2024-2026
- PhD Fellowships: Z. Mushtaq, 2025-2028 (FI); F. Fariha, 2025-2029 (FPI); R. Sharma, 2025-2028 (IFUdG); A. Bhaskaran, 2023-2026 (IFUdG); R. Mollfulleda, 2022-2027 (FPI); F. Ahsan, 2022-2026 (FI)
- Unlimited site license ADF program package (developer, SCM), 2002-present

Furthermore, I'm official collaborator in a NSF project (I. Garcia-Bosch).
Previously funded grants include a SWAFS grant, a FetOpen grant, COST Action, Marie Curie Fellowships x2, Juan de la Cierva Fellowships x2, Europa Excelencia, *Proyectos de Excelencia I+D* (including FPI fellowships), MICINN Infrastructure grants, H2020 exchange projects (HPC-Europa3), industry grants (Repsol, Lucta), UdG grants for research and personnel, and FP7 grants (CIG, IRSES). Furthermore, I've been official collaborator in NSF and NIH grants (I. Garcia-Bosch), ERC-StG grant (A. McDonald) and BSC-RES data storage projects of collaborators.

One Beatriu de Pinós (V. Elumalai) and one FI PhD fellowship (Y. Balmohammadi) were cancelled due to personal circumstances of the candidates.

## 8 Supervision, examinations, evaluation, and promotion panels

I have engaged with different forms of supervision ranging from tutoring secondary-school scholars, to Erasmus, Bachelor, Master, PhD students and postgrads. Since 2009 I supervised more than 15 postdocs and 30 PhD, Master, undergraduate, and summer students. I frequently act as external PhD examiner in Spain and abroad, both as reading committee and tribunal member. I form(ed) part of DFG Panels, FWO Evaluation Panel for Chemistry (Flanders), LaCaixa panels for PhD and postdoc fellowships, Spanish national evaluation agency (ANEP) for postdoctoral fellowships and short-term visits of staff members. I have been member of the BSC/RES Users Committee, expert for evaluations of research proposals of AEI, ANEP, DFG, ERC, FWO, FWF, GACR, LaCaixa, MSCA, NWO, PRACE, Royal Society, SARA, SNF, and member of staff promotion committees for Austria, Czech Republic, France, Ireland, Norway, Spain, UK, and USA.

## 9 Selected administrative duties and committee work

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|---|---|
| 04/2023 – present | Member of Steering Committee for Academia Europaea Barcelona Knowledge Hub |
| 04/2018 – present | Founding Member and Vice-President *Grupo Especializado Química y Computación* (GEQC) of Spanish Chemical Society (RSEQ) |
| 06/2023 – 12/2025 | Member of the SAPEA Working Group related to the work package on 'Early and mid-career researchers' (WP6) |
| 06/2024 – 11/2024 | Member of Access Committee of BSC-CNS/RES |
| 10/2019 – 08/2024 | Member of Advisory Council of Young Academy of Europe |
| 06/2019 – 02/2024 | Member of UdG committee for Communication |
| 04/2018 – 08/2023 | Founding Member and Vice-President Quantum-Bio·Inorganic Chemistry (QBIC) Society |
| 03/2012 – 06/2023 | Member of UdG Claustre (equivalent to Senate) |
| 09/2019 – 06/2023 | Member of UdG Steering Committee for HRS4R |
| 05/2017 – 12/2022 | Member Higher Education, Research and Culture in European Societies (HERCulES) group |
| 01/2018 – 09/2020 | Member of UdG committees for Quality Control, International Policy |
| 03/2016 – 07/2020 | Member Management Board, Catalonian Research Network XRQTC |
| 11/2018 – 10/2019 | Outgoing Chair Young Academy of Europe |
| 04/2014 – 09/2019 | Member of *Comité de Usuarios de la Red Española de Supercomputación* |
| 03/2018 – 09/2019 | External Scientific Advisory Board, Foster Plus, www.fosteropenscience.eu |
| 01/2017 – 11/2018 | Chair of the Young Academy of Europe (YAE) and YAE representative at Academia Europaea Board of Trustees, and at Academia Europaea Communications Group |
| 07/2015 – 12/2017 | Member of UdG University Council, UdG Committees for Research and Doctorate Studies; Personnel; International Policy |

## 10 Editorial responsibilities

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|---|---|
| 06/2022 – present | Collection Advisor Computational Chemistry, Open Research Europe (EC) |
| 04/2022 – present | Community Gateway Advisor Inorganic Chemistry, ORE (EC) |
| 05/2021 – present | Member Editorial College *SciPost Chemistry* |
| 07/2020 – present | Editor *Inorganica Chimica Acta* |
| 09/2015 – present | Member Editorial Board *Journal of Molecular Graphics and Modelling* |
| 03/2014 – present | Member Editorial Board *Journal of the Serbian Chemical Society* |
| 03/2016 – 06/2020 | Member Editorial Board *Inorganica Chimica Acta* |
| 10/2015 – 10/2016 | Associate Editor *RSC Advances* |
| 06/2013 – 12/2015 | Editor first text-book on spin states, "Spin states in biochemistry and inorganic chemistry: Influence on Structure and Reactivity" (Wiley, 2015) |
| 06/2012 – 06/2013 | Guest editor special issues *Current Organic Chemistry* and *Current Inorganic Chemistry* |
| Reviewer activity | See: https://publons.com/a/1212468/ and www.bit.ly/MSwartORCID |

## 11 Links with industry

Since 1998 I am developer of the Amsterdam Density Functional program, maintained by SCM (Software for Chemistry & Materials, Amsterdam), with developer (unlimited) site license. Apart from SCM I had projects with industry regarding food taste receptors (Lucta) and catalysis (Repsol).

**12 Academic leadership**

Selected Conference, Seminar, and Colloquium organisation:

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|---|---|
| 07/2026 | Coordinator of compchem sessions at 18th European Bioinorganic Chemistry Conference (Groningen, NL) |
| 06/2026 | "Electronic and molecular structure – methods and modelling" Symposium at 46th International Coordination Chemistry Conference (Odense, DK) |
| 07/2024 | "Coordination Chemistry of High-Valent Oxidants" Symposium at 45th International Coordination Chemistry Conference (Fort Collins, CO, USA) |
| 06/2023 | "Chemical Reactivity: Computational Methods and Applications" Symposium at XXXIX Reunión Bienal RSEQ (Zaragoza, ES) |
| 05/2023 | International Symposium on “Publishing in Academia: Digital Challenges”, Academia Europaea and Wenner-Gren Foundations (Stockholm, SE) |
| 04/2023 | "30 years IQC(C)" (Girona, ES) |
| 04/2018 | Girona Seminar on Predictive Catalysis: Transition-Metal Reactivity by Design (gender-balanced invited speaker list); including support for Young Researchers Symposium (Girona, ES) |
| 06/2017 | "Progress in Theoretical Chemistry: Biomolecules and Materials" Symposium at XXXVI Reunión Bienal RSEQ (Sitges, ES) |
| 07/2016 | Summer Training School COST Action CM1305 (ECOSTBio) (Groningen, NL) |
| 04/2016 | Girona Seminar on Predictive Catalysis: Transition-Metal Reactivity by Design, with gender-balanced invited speaker list, (Girona, ES) |
| 07/2015 | Summer Training School COST Action CM1305 (ECOSTBio) (Groningen, NL) |
| 06/2015 | XXXI Meeting of the XRQTC Research Network (Girona, ES) |
| 09/2012 | CECAM/ESF Workshop on "Spin states in biochemistry and inorganic chemistry", highlighted in Nature Chem. 2013, 5, 7-9 (Zaragoza, ES) |
| 06/2010 – present | Annual DFT Popularity Poll, see guest post on guest post on Nature Chemistry's Sceptical Chymist blog, https://bit.ly/5yearsDFTPoll |

International scientific committee:

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|---|---|
| 06/2026 | 46th International Conference on Coordination Chemistry (Odense, DK) |
| 04/2023 | 2023 FrenchBIC annual meeting (Logonna-Daoulas, FR) |
| 10/2021 | HPC-Europa3 Transnational Access Meeting (Amsterdam, NL) |
| 04/2014 – 04/2018 | Chair of COST Action CM1305 (ECOSTBio); Supervision of activities and co-organization of meetings in Girona (09/2014), Marseille (01/2015), Warwick (04/2015), Belgrade (08/2015), Prague (04/2016), Brest (07/2016), Kraków (09/2016), Lisbon (03/2017), Dublin (12/2017), Berlin (04/2018) |

**13 Main collaborations**

| | |
|---|---|
| Transition-metals: | Wesley Browne (Groningen), Isaac Garcia-Bosch (Carnegie Mellon), Maja Gruden (Belgrade), Aidan McDonald (Trinity Dublin), Christine McKenzie (SDU Odense), Larry Que (Minnesota), Moniek Tromp (Groningen) |
| Nanomaterials: | Nicole Grobert (Oxford), Sílvia Osuna (Girona) |
| Solid state: | Pier Philipsen (SCM), Jörg Wagler (Freiberg) |

**14 Academic accreditations for Full Professor**

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|---|---|
| 01/2023 | Certificado I3 del Programa de Incentivación de la Incorporación e Intensificación de la Actividad Investigadora, Ministerio de Universidades |
| 10/2021 | Acreditació de Recerca Avançada de l'Àmbit de Ciències, Agència per a la Qualitat del Sistema Universitari de Catalunya |

**15 Supervision of PhD, Master and TFG theses**

PhD theses:

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|---|---|
| 06/2029 | Fiza Fariha – "Chiral confined spaces for applications in asymmetric catalysis and chiroptical materials" |
| 09/2028 | Zanira Mushtaq – "A computational study on chiral confined spaces in host-guest complexes" |
| 03/2028 | Rupal Sharma – "Computational design of metalloenzymes" |
| 07/2027 | Jonnely Luizaga – "QM/MM simulations for enzyme design" |
| 04/2027 | Rosa Mollfulleda – "Organometallic and oxidation chemistry, (re)design of methods and ligands" |
| 10/2026 | Athul Santha Bhaskaran – "Boron Nitride Nanomaterials and Density Functional methods" |
| 07/2026 | Faiza Ahsan – " Functionalization of inert C-H bonds by transition metal complexes: a computational chemistry study" |
| 10/2023 | Frederico Martins – "Density functional theory to the rescue of transition-metal chemistry" (http://hdl.handle.net/10803/689726) |
| 12/2021 | Lorenzo D'Amore – "Enzymatic and bioinspired iron oxidation chemistry: a computational study" (http://hdl.handle.net/10803/674109) |
| 02/2021 | Miguel Angel María-Solano – "Computational studies of the conformational landscape of allosteric and enantioselective enzymes" (http://hdl.handle.net/10803/671771) |
| 08/2020 | Filip Vlahovic – "Application of methods based on Density Functional Theory, for studying electronic states of aqua- and oxo- first row transition metal complexes" (https://www.chem.bg.ac.rs/pz/rfile.py?s=3&q=2553&n=disertacija.pdf) |
| 12/2018 | Adrià Romero-Rivera – "Computational studies of enzymatic and biomimetic catalysts" (http://hdl.handle.net/10803/666175) |
| 05/2018 | Stepan Stepanovic – "Density functional approximations for spin state energetics in transition-metal complexes" (http://www.chem.bg.ac.rs/vesti/1875/disertacija.pdf) |
| 11/2017 | Abril Castro – "Computational study of nuclear magnetic resonance shielding constants" (http://hdl.handle.net/10803/565597) |
| 03/2010 | Sílvia Osuna – "Theoretical studies of the exohedral reactivity of fullerene compounds" (http://hdl.handle.net/10803/7944) |
| 07/2009 | Mireia Güell – "Theoretical studies of systems of biochemical interest containing Fe and Cu transition metals" (http://hdl.handle.net/10803/7941) |

Master theses:

| | |
|---|---|
| 07/2023 | Jonnely Luizaga – "Resolving the controversy between machine learning and experiment" |
| 07/2022 | Rosa Mollfulleda – "Mechanism of catalytic thioetherification from nickel complex with N-heterocyclic ligand" |
| 07/2014 | Adrià Romero-Rivera – "Mechanism of action of Salen-Manganese antioxidant complexes: The Catalase reaction to neutralize reactive oxygen species" |
| 09/2008 | Lluís Armangué – "Estudi teòric sobre la caracterització de Citocroms C utilitzant NMR" |
| 06/2007 | Sílvia Osuna – "Study of the Diels-Alder reaction on endohedral fullerenes" (*Diploma d'estudis avançats*) |
| 04/2005 | Tushar van der Wijst – "Proper descriptions of the interaction between stacked DNA bases and Watson-Crick base pairs using density functional theory" |

TFG Final degree theses:

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|---|---|
| 07/2024 | Josep Arbusà – "Oxidation chemistry of model complexes" |
| 07/2023 | Dani Romero – "Reactivity of endohedral $C_{36}$ fullerenes" |
| 07/2022 | Joan Manel Maneu-Garcia – "NMR study of cyclic imino ether isomers" |
| 07/2021 | Jonnely Luizaga – "DFT study of the mechanism of an aldol reaction followed by [5+1] annulation to afford tetralines" |
| 07/2021 | Rosa Mollfulleda – "Punts de creuament de mínima energia dels hidrurs de ferro, cobalt i níquel iònics amb metà" |
| 07/2021 | Soufyane El Baizi – "Palladium(II)/Lewis Acid-Catalyzed Oxidative Olefination/ Annulation of N-Methoxybenzamides: Identifying the Active Intermediates through NMR Characterizations" |
| 07/2020 | Nadina Fradera – "Entenent el gust Umami a nivell biomolecular" |
| 07/2017 | Jaume Puigdefàbregas – "Un Estudi Computacional i teòric sobre els Complexos Ferro-Oxo" |
| 06/2017 | Laura Timonet – "Estructura del receptor humà umami i l'optimització dels seus substrats" |
| 06/2016 | Eudald Gubert – "Dinàmica molecular de complexos de ferro de spin-crossover" |
| 06/2013 | Adrià Romero-Rivera – "Study of reactivity on endohedral fullerene $C_{36}$ through theoretical chemistry" |

**16 Teaching**

ICREA Research Professors are not allowed to do teaching, unless the university offers an additional contract, which I had since 2018 as Associate Professor (annually renewed) until Dec. 2024. In Dec. 2024, this was transformed into a permanent part-time (10%) full professor position, in addition to my permanent ICREA position.

Courses taught (yearly between 3 and 3.5 credits):

- Open Science for Researchers (Grad School, 1.0 credits)
  - 2025-present
- Open Science (Grad School, 0.5 credits)
  - 2018-2024
- Biomolecular design (4$^{th}$ year Chemistry/Biotechnology degrees, 2 credits)
  - 2018-present
- Science Communication (MSc course MACMoM, 0.5 credits)
  - 2018-2019; 2019-2020; 2020-2021
- Density Functional Theory principles and applications (summer school ECOSTBio COST Action)
  - 2016, Groningen; 2017, Groningen
- Density Functional Theory and ADF (International Intensive Course of European Master in Theoretical Chemistry and Computational Modelling)
  - 2013, Madrid; 2015, Groningen

Additionally, I organized ADF workshops at CESCA Supercomputing Center Barcelona (2008), QUITEL conference Riviera Maya, México (2011) and contributed to SurfSara workshops (2021, 2022) with a course on multi-level QM/MM and QM/QM methods. In January 2026 I organized a one-month mini-course on “Use of Python in chemistry” for my research group.

**Additional appointment**

Starting in Spring 2026 I will be appointed Honorary Full Professor at the Zernike Institute for Advanced Materials of the University of Groningen. This appointment will be focused on teaching Theoretical Chemistry in BSc, MSc and PhD courses.

**Papers**
DOIs, #OpenAccess and #OpenData: www.marcelswart.eu/publ/

[185] P.M. Crossland, B. Chandra, S. Banerjee, C. Abelson, Y. Guo, M. Swart* and L. Que*
"Mimicking sMMOH Chemistry: Trapping the $Sc^{3+}$-bound Nonheme $Fe^{III}$-O-O-$Fe^{III}$ Adduct Prior to Its Conversion into an $Fe^{IV}_2(\mu\text{-}O)_2$ Core"
*Chem. Sci.* **2025**, *16*, 19608-19613 [+back-cover]

[184] D.R. Duijnstee, M. Di Berto Mancini, C.M. de Roo, D. Unjaroen, M. Tromp, R. Hage, W.R. Browne* and M. Swart*
"Ligand Driven Heterolytic O-O Bond Cleavage in a non-haem Phenolato-Fe(III)-OOH Complex to Yield a Formal Fe(V)=O intermediate"
*Dalton Trans.* **2025**, *54*, 14566-14577

[183] A. Inchausti, R. Mollfulleda, M. Swart, J. Perles, S. Herrero, V.G. Baonza, M. Taravillo and A. Lobato*
"Chemical tuning of the electronic structure in diruthenium compounds"
*J. Phys. Chem. Lett.* **2025**, *16*, 10000-10008

[182] P-Y. Lee, B.M. Maciejewska, M.J. Cross, C.M. van Beek, C.N. Brodie, A.S. Bhaskaran, G.T. Tebbutt, R.M. Schofield, S.J. Page, E. Darnbrough, M. Swart, A.S. Weller* and N. Grobert*
"A straightforward route to hexagonal-boron nitride fibers"
*Adv. Compos. Hybrid Mater.* **2025**, *8*, 392

[181] B. Chandra, C. Li, M. Ansari, J. Xiong, A. Lovstedt, Y. Guo, M. Swart* and L. Que*
"Million-Fold Activation of C¬H Bonds by Fluorinated Non-heme FeIV=O Complexes via Second Sphere Equatorial Substitution and Catalytic Epoxidation to Boot"
*ACS Catal.* **2025**, *15*, 17361-17372 [+supplementary cover]

[180] A. Santha Bhaskaran, S. Osuna* and M. Swart*
"Computational exploration of Xe dimers inside fullerene cages"
*J. Phys. Chem. A* **2025**, *129*, 7609-7616

[179] O.R. Kelly, B. Twamley, M. Swart and A.R. McDonald*
"Electrostatic Fields Induce Accelerated Proton Coupled Electron Transfer Rates in Chlorophyll Model Compounds"
*J. Am. Chem. Soc.* **2025**, *147*, 29399-29412

[178] F. Ahsan, M. Ansari, J.E.M.N. Klein and M. Swart*
"Characterization of σ and π Reaction Channels in Hydrogen Atom Transfer Reactions"
*J. Inorg. Biochem.* **2025**, *272*, 112989

[177] D. Hebert, A. Puri, D. Ye, A. McAninch, A. Chisholm, M. Siegler, M. Swart* and I. Garcia-Bosch*
"Synthesis and Characterization of Copper Complexes Featuring a Redox-Active ONO Ligand in Three Molecular Oxidation States"
*Inorg. Chem.* **2025**, *64*, 11204-11218

[176] M. Swart* and I. Garcia-Bosch*
"Characterization of Three Intermediates in an Unusual Copper-Dependent Enzyme"
*ACS Cent. Sci.* **2025**, *11*, 656-658

[175] J. Chen, A.S. Sardjan, C.M. De Roo, M. Di Berto Mancini, A. Draksharapu, D. Angelone, R. Hage, M. Swart* and W.R. Browne*
"Generation of $[(N4Py)Fe(IV)=O]^{2+}$ through Heterolytic O-O Bond Cleavage in $[(N4Py)Fe(II)(OOH)]^{+}$"
*Inorg. Chem.* **2025**, *64*, 9408-9417

[174] M. Di Berto Mancini,* C.M. De Roo, A.S. Sardjan, R. Hage, G. Olivo, O. Lanzalunga, M. Swart and W.R. Browne*
"A transient highly reactive Fe(IV)=O species revealed through the interference by $O_2$ in the activation of organic peracids by $[(N4Py)Fe(II)]^{2+}$"
*ACS Catal.* **2025**, *15*, 7482-7495

[173] E.J. Baerends,* N.F. Aguirre, N.D. Austin, J. Autschbach, F.M. Bickelhaupt, R. Bulo, C. Cappelli, A.C.T. van Duin, F. Egidi, C. Fonseca Guerra, A. Förster, M. Franchini, F.T.P.M. Goumans, T. Heine, M. Hellström, C.R. Jacob, L. Jensen, M. Krykunov, E. van Lenthe, A. Michalak, M.M. Mitoraj, J. Neugebauer, V.P. Nicu, P. Philipsen, H. Ramanantoanina, R. Rüger, G. Schreckenbach, M. Stener, M. Swart, J.M. Thijssen, T. Trnka, L. Visscher, A. Yakovlev, and S.J.A. van Gisbergen*
"The Amsterdam Modeling Suite"
*J. Chem. Phys.* **2025**, *162*, 162501

[172] G.J. Linker, M. Swart* and P.Th. van Duijnen
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*Int. J. Quant. Chem.* **2025**, *46*, e70032 [+cover]

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