

Curriculum Vitae

Marcel Swart

Professor Dr. FYAE FRSC MAE

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1 Personal details

IQCC Institute and Department of Chemistry, University of Girona (UdG)

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2 Appointments

09/2009 – present ICREA Professor at IQCC Institute, University of Girona
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

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

4 Honours and awards

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; [€]cancelled^{COVID19})

- 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)
~~08/2020 * 15th European Biologic Inorganic Chemistry conference (EuroBic), Reykjavik (IS) [€]~~
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)
05/2013 * 4th International Conference on Biological Inorganic Chemistry (CANBIC-4), Parry
Sound (CAN)
09/2008 ** 9th European Biological Inorganic Chemistry (EuroBic) conference, Wroclaw (PL)

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

Hylleraas Center, Univ. Oslo (2023) – SDU Odense (2023) – IIT Roorkee (2021^{online}) – LMU Munich
(2021^{online}) – Univ. Oxford (2020^{online}) – Univ. Sheffield (2020^{online}) – Univ. Bayreuth (2020) – Univ.
Helsinki (2019) – Univ. Leuven (2019) – SD Univ. Odense (2019) – UvA Univ. 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	<i>Panel SAPEA Workshop, Tallinn (EE) (cancelled, family circumstances)</i>
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. 3m 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 "CorrFunc", 121.000€ + FPI (PI), 2021-2024
- Project UdG Promotors2021 IQCC, 60.000€ (PI as Director IQCC), 2022-2024
- PhD Fellowships: IFUdG (UdG) A. Bhaskaran, 69.500€ (PI), 2023-2026; FPI (AEI/MCIU) R. Mollfulleda, 92.750€ (PI), 2022-2026; FI (GenCat) F. Ahsan, 75.130€ (PI), 2022-2025
- Unlimited site license ADF program package (developer, SCM), 2002-present

Furthermore, I'm official collaborator in NSF (I. Garcia-Bosch) and BSC-RES data storage projects of collaborators.

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).

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 the 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 Czech Republic, Ireland, Norway, Spain, UK, and USA.

9 Selected administrative duties and committee work

05/2024 –	Member of <i>Comité de Acceso</i> de BSC-CNS
06/2023 – present	Member of the SAPEA Working Group related to the work package on ‘Early and mid-career researchers’ (WP6)
10/2019 – 10/2024	Member of Advisory Council of Young Academy of Europe
06/2019 – present	Member of UdG committee for Communication
04/2018 – present	Founding Member and Vice-President <i>Grupo Especializado Química y Computación</i> (GEQC) of Spanish Chemical Society (RSEQ)
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, Catalanian Research Network XRQTC
11/2018 – 10/2019	Outgoing Chair Young Academy of Europe
04/2014 – 09/2019	Member of <i>Comité de Usuarios de la Red Española de Supercomputación</i>
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 Committee for Research and Doctorate Studies, UdG Committee for Personnel, UdG Committee for International Policy

10 Editorial responsibilities

06/2022 – present	Collection Advisor Computational Chemistry, Open Research Europe (EC)
04/2022 – present	Community Gateway Advisor Inorganic Chemistry, Open Research Europe (EC)
05/2021 – present	Member Editorial College <i>SciPost Chemistry</i>
07/2020 – present	Editor <i>Inorganica Chimica Acta</i>
09/2015 – present	Member Editorial Board <i>Journal of Molecular Graphics and Modelling</i>
03/2014 – present	Member Editorial Board <i>Journal of the Serbian Chemical Society</i>
03/2016 – 06/2020	Member Editorial Board <i>Inorganica Chimica Acta</i>
10/2015 – 10/2016	Associate Editor <i>RSC Advances</i>
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 <i>Current Organic Chemistry</i> and <i>Current Inorganic Chemistry</i>
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 (Luacta) and catalysis (Repsol).

12 Academic leadership

Selected Conference, Seminar, and Colloquium organisation:

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:

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 Academic accreditations for Full Professor

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

14 Main collaborations

Transition-metal chemistry: Wesley Browne (Groningen), Alicia Casitas (Marburg), 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 physics/chemistry: Pier Philipsen (SCM), Jörg Wagler (Freiberg)

15 Supervision of PhD, Master and TFG theses

PhD theses:

- 10/2026 Jonnelly Luizaga – "QM/MM simulations for enzyme design"
- 07/2026 Rosa Mollfulleda – "Organometallic and oxidation chemistry, (re)design of methods and ligands"
- 01/2026 Athul Santha Bhaskaran – "Boron Nitride Nanomaterials and Density Functional methods"
- 07/2025 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"
- 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 Jonnelly 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:

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 have since 2018 as Associate Professor (annually renewed).^a Currently, the UdG is in the process of transforming this into a permanent part-time full professor position, in addition to my permanent ICREA position.

Courses taught (yearly between 3 and 3.5 credits):^b

- Open Science (Grad School, 0.5 credits)
 - 2018-present
- Biomolecular design (4th 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

a) at the Chemistry Dept. of the UdG there have been since 2006 typically 25+ staff members (including currently 11 permanent computational researchers and 2 senior computational postdocs) that are obliged to teach a certain amount of credits, which makes it difficult for ICREA Professors to obtain the possibility to start teaching.

b) additional credits are earned for teaching in English (20%), and 0.25 credit per final degree project that has been supervised.

Additionally, I organized ADF workshops at CIESCA 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.

Papers

DOIs, #OpenAccess and #OpenData: www.marcelswart.eu/pub/

- [159] B. Chandra, F. Ahsan, Y. Sheng, M. Swart,* L. Que, Jr.*
"A Tale of Two Topological Isomers: Uptuning $[\text{Fe}^{\text{IV}}(\text{O})(\text{Me}_4\text{cyclam})]^{2+}$ for Olefin Epoxidation"
Proc. Natl. Acad. Sci. USA **2024**, in press (under embargo)
- [158] C.M. de Roo, A.S. Sardjan, R. Postmus, M. Swart, R. Hage,* W.R. Browne*
"Reaction of $(\text{N}_4\text{Py})\text{Fe}$ with H_2O_2 and the relevance of its $\text{Fe}(\text{IV})=\text{O}$ species during and after H_2O_2 disproportionation"
ChemCatChem **2024**, DOI 10.1002/cctc.202301594
- [157] A. Puri, A. McAninch, S. Shu, K. Rajabimoghadam, M.A. Siegler, M. Swart,* I. Garcia-Bosch*
"Geometric Control of Cu, Ni and Pd Complexes in the Solid State via Intramolecular H-Bonding Interactions"
Inorg. Chim. Acta **2024**, 561, 121844
- [156] R. Kumar, F. Ahsan, A. Awasthi, M. Swart,* A. Draksharapu*
"Generation of Ru(III)-hypochlorite with resemblance to heme dependent haloperoxidase enzyme"
Dalton Trans. **2023**, 52, 12552-12559
- [155] E. Jaimes-Romano, H. Valdés,* S. Hernández-Ortega, R. Mollfulleda, M. Swart,* D. Morales-Morales*
"C-S Couplings Catalyzed by Ni(II) Complexes of the Type $[(\text{NHC})\text{Ni}(\text{Cp})(\text{Br})]$ "
J. Catal. **2023**, 426, 247-256
- [154] .F. Martins and M. Swart*
"Electronic properties and redox chemistry of N confused metalloporphyrins"
J. Porphyr. Phthalocya. **2023**, 27, 1320-1329
- [153] E. Díaz-Cervantes, J. Robles, M. Solà and M. Swart*
"The peptide bond rupture mechanism in the serine proteases: an in silico sequential scale models study"
Phys. Chem. Chem. Phys. **2023**, 25, 8043-8049
- [152] M. Bhadra*, T. Albert, A. Franke, V. Josef, I. Ivanović-Burmazović, M. Swart, P. Moëne-Loccoz*, K. Karlin*
"Reductive Coupling of Nitric Oxide by Cu(I): Stepwise Formation of Mono and Dinitrosyl Species en route to a Cupric Hyponitrite Intermediate"
J. Am. Chem. Soc. **2023**, 145, 2230-2242
- [151] T. Wu, K. Rajabimoghadam, A. Puri, D.D. Hebert, Y.L. Qiu, S. Eichelberger, M.A. Siegler, M. Swart*, M.P. Hendrich* and I. Garcia-Bosch*
"A $4\text{H}^+/4\text{e}^-$ Electron-Coupled-Proton Buffer Based on a Mononuclear Cu Complex"
J. Am. Chem. Soc. **2022**, 144, 16905-16915
- [150] C. Souilah, S.A.V. Jannuzzi, D. Demirbas, S. Ivlev, M. Swart, S. DeBeer and A. Casitas*
"Synthesis of Fe(III) and Fe(IV) Cyanide Complexes Using Hypervalent Iodine Reagents as Cyano-Transfer One-Electron Oxidants"
Angew. Chem. Int. Ed. **2022**, 61, e202201699
- [149] A. Brinkmeier, K.E. Dalle, L. D'Amore, R.A. Schulz, S. Dechert, S. Demeshko, M. Swart*, and F. Meyer*
"Modulation of a μ -1,2-Peroxo Dicopper(II) Intermediate by Strong Interaction with Alkali Metal Ions"
J. Am. Chem. Soc. **2021**, 143, 17751-17760
- [148] K. Warm, I. Monte Pérez, U. Kuhlmann, P. Hildebrandt, E. Farquhar, M. Swart*, and K. Ray*
"Stable, but still reactive - investigations on the effects of Lewis acid binding on copper nitrene intermediates"
Z. Anorg. Allg. Chem. **2021**, 647, 1495-1502
- [147] K. Warm, A. Paskin, U. Kuhlmann, E. Bill, M. Swart, M. Haumann, H. Dau, P. Hildebrandt and K. Ray*
"A Pseudotetrahedral Terminal Oxoiron(IV) Complex: Mechanistic Promiscuity in C-H bond Oxidation Reactions"
Angew. Chem. Int. Ed. **2021**, 60, 6752-6756
- [146] P. Vermeeren, T. Hansen, P. Jansen, M. Swart, T.A. Hamlin*, and F.M. Bickelhaupt*
"A Unified Framework for Understanding Nucleophilicity and Protophilicity in the $\text{S}_{\text{N}}2/\text{E}2$ Competition"
Chem. Eur. J. **2020**, 26, 15538-15548
- [145] L. D'Amore, L. Belpassi, J.E.M.N. Klein and M. Swart*
"Spin-Resolved Charge Displacement Analysis as Intuitive Tool for the Evaluation of cPCET and HAT Scenarios"
Chem. Commun. **2020**, 56, 12146-12149

- [144] M. Swart*
"Bond orders in metalloporphyrins"
Theor. Chem. Acc. **2020**, *139*, 160
- [143] O.A. Stasyuk*, M. Solà, M. Swart, C. Fonseca Guerra, T.M. Krygowski, H. Szatyłowicz*
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