

Prof. Dr. Marcel Swart FRSC
Chair of Young Academy of Europe
ICREA Research Professor at
Institut de Química Computacional i Catàlisi (IQCC)
Universitat de Girona
<http://www.marcelswart.eu>



Education and training

- 1998-2002 PhD study, University of Groningen (NL)
Supervision: Prof. H.J.C. Berendsen, Prof. G.W. Canters, Prof. J.G. Snijders[†]
PhD ceremony: 10th September, 2002
- 1999 European Summer school in Quantum Chemistry, Tjörnarp (SE)
1998 Fifth Sostrup Summer School on Quantum Chemistry, Århus (DK)
1997-2001 Annual winter school Theoretical Chemistry & Spectroscopy, Han-sur-Lesse (BE)
1990-1996 Undergraduate and Master study Chemistry, University of Groningen (NL)

Professional experience

- 2015-now Director IQCC
2009-now ICREA Research Professor, Institute of Computational Chemistry and Catalysis (IQCC),
University of Girona (ES) (*permanent position*)
Project: “Spinning around in transition-metal chemistry”
- 2006-2009 ICREA-Júnior Researcher, Institute of Computational Chemistry, University of Girona (ES)
2004-2006 Postdoc researcher, Theoretical Chemistry, VU University Amsterdam (NL)
Project: “Density Functional Theory investigation of the structure of DNA”,
Supervision: Prof. F.M. Bickelhaupt
- 2002-2004 Postdoc researcher, Organic and Inorganic Chemistry, VU University Amsterdam (NL) Project:
“Spin states and QM/MM Study of catalytic cycle of cytochrome P450”, Supervision: dr. A.W.
Ehlers, Prof. K. Lammertsma
- 1998-2002 PhD study, Theoretical Chemistry, University of Groningen (NL)
Thesis: “Density Functional Theory Applied to Copper Proteins”,
Supervision: Prof. H.J.C. Berendsen, Prof. G.W. Canters, Prof. J.G. Snijders[†]
- 1995-1996 Master study, Organic Chemistry, University of Groningen (NL)
Thesis: “Reflections on the DRF model. From atomic polarizabilities to potentials of mean
force”, Supervision: dr. P.Th. van Duijnen

Supervision of research visits and theses

- Supervision of short research stays (2-10 months) of 11 high-school/Master/PhD students, 3 postdocs and 3 visiting professors (2009-now)
- A. Romero-Rivera, “Mechanism of action of Salen-Manganese antioxidant complexes: The Catalase reaction to neutralize reactive oxygen species”, July 2014, Girona (Master thesis, director)
- A. Romero-Rivera, “Study of reactivity on endohedral fullerene C₃₆ through theoretical chemistry”, June 2013, Girona (Undergraduate thesis, director)
- S. Osuna Oliveras, “Theoretical studies of the exohedral reactivity of fullerene compounds”, March 2010, Girona (PhD thesis, director), *awarded the Premi Extraordinari de Doctorat 2010*
- M. Güell Serra, “Theoretical studies of systems of biochemical interest containing Fe and Cu transition metals”, July 2009, Girona (PhD thesis, co-director), *awarded the Premi Extraordinari de Doctorat 2009*
- Ll. Armangué Fraixinó, “Estudi teòric sobre la caracterització de Citocroms C utilitzant NMR”, September 2008, Girona (Master thesis, director)
- S. Osuna Oliveras, “Study of the Diels-Alder reaction on endohedral fullerenes”, June 2007, Girona (*Diploma d'estudis avançats* midterm PhD thesis, director)
- T. van der Wijst, “Proper descriptions of the interaction between stacked DNA bases and Watson-Crick base pairs using density functional theory”, April 2005, Amsterdam (Master thesis, co-supervisor)

Publications and citations

- Articles: 131; Book chapters: 8 (<http://www.marcelswart.eu/publ>)
- H-index: 33 (ISI-WoS), 33 (Scopus), 38 (Google Scholar)
- Citations: >4000 (ISI-WoS, www.goo.gl/753OUo), >4050 (Scopus, www.goo.gl/1A1SNp), >5650 (Google Scholar, www.goo.gl/LfUzva)

Current Funding ID

- PhD Scholarship (FPI) for L. D'Amore, ca. €47.700, Sep. 2016- Aug. 2019 (**researcher in charge**)
- PhD Scholarship (FPI) for M.A. Maria Solano, ca. €92.750, May 2016- May 2020 (**researcher in charge**)
- “Química predictiva a l'espai confinat” (MPCUdG2016), R&D project Univ. Girona, €345.000, Jan. 2016- Dec. 2018 (**PI**)
- “SpinEnzymeCat” (CTQ2014-59212/BQU), R&D project MINECO, Spain, €116.160 (+PhD scholarship), Jan. 2015-Dec. 2017 (**PI**)
- Marie Curie postdoc position dr. F. Feixas, EU-H2020, €158.122, May 2015-May 2017, (**researcher in charge**)
- PhD scholarship (GenCat) for A. Romero-Rivera, “*Density functional and molecular dynamics study on a 2,3-dioxygenase copper enzyme*”, €54.530, Feb. 2015-Feb. 2018 (**researcher in charge**)
- ECOSTBio COST Action (CM1305), ca. €590.000, April 2014-April 2018 (**coordinator, Action Chair**)
- Career Integration Grant dr. S. Osuna, EU-FP7, €100.000, March 2014-March 2018 (**researcher in charge**)
- PhD Scholarship (FPI, BES-2012-052792) for A. Castro, “*Nuclear magnetic resonance of organic molecules, fullerenes and heme proteins*”, €70.408, May 2013-May 2017 (**researcher in charge**)

Past Funding ID (since 2008)

- PI/Researcher in charge/(Co-)Investigator for two PhD-scholarships, four postdoc positions, and GenCat/MICINN/MINECO R&D projects, >€1.100.000, 2008-2015
- Three projects with industry, €66.000, 2008-2016
- ESF/CECAM financial support for organization Workshop in Zaragoza, €21.000, Sept. 2012
- Supercomputer research grants (4 months) on Barcelona Supercomputing Center (BSC) and Red Española de Supercomputación, Jan. 2007-Feb. 2016: 44 (total: **4.39 Mhours as PI**, 3.89 Mhours as co-investigator)

International honors and awards

- Elected Fellow of the Royal Society of Chemistry (Nov. 2015)
- Elected member of Young Academy of Europe (Oct. 2014, upon invitation)
- Molecular Graphics and Modelling Society (MGMS) Silver Jubilee Prize 2012
Prize committee: “This award recognises his development of new computational chemistry programs, design of new research tools and application to (bio)chemical systems that are highly relevant for society and science. Competition for the prize was very strong this year, but Dr Swart's submission was truly outstanding.” (www.mgms.org)
- ICREA-Senior position awarded, 2009- (permanent position)
- Six journal covers, one VIP paper and two Highly-Cited papers (ISI Essential Science Indicators)
- Selected as *Promising young chemist* to contribute to a special issue for the 40th anniversary of *Inorganica Chimica Acta*, titled “Inorganic Chemistry - The Next Generation”
- ICREA-Júnior position awarded, 2006-2011
- Young Scientist Excellence Award 2005, International Conference of Computational Methods in Sciences and Engineering (www.iccmse.org)

National prizes and awards under my supervision

- *Premi Extraordinari de Doctorat en Química 2010* for Silvia Osuna
- *Premi Extraordinari de Doctorat en Química 2009* for Mireia Güell

Major collaborations

- Prof. F.M. Bickelhaupt, Dept. Chemistry, VU University Amsterdam, The Netherlands (2004-)
- Prof. P.Th. van Duijnen, Dept. Chemistry, University of Groningen, The Netherlands (1995-)
- Dr. C. Fonseca Guerra, Dept. Chemistry, VU University Amsterdam, The Netherlands (2004-)
- Dr. M. Gruden-Pavlovic, Dept. Chemistry, University of Belgrade, Serbia (2012-)
- Dr. L. Kamerlin, Dept. Biochemistry, Uppsala, Sweden (2013-)
- Dr. A. McDonald, Trinity College, Dublin, Ireland (2014-)
- Prof. F. Meyer, University Göttingen, Germany (2015-)
- Dr. K. Ray, Humboldt University, Berlin, Germany (2014-)
- Prof. W.R. Browne, Dept. Chemistry, University of Groningen, The Netherlands (2015-)

Organization conferences, courses and workshop

- Main Organizer Girona Seminar 2018: “Predictive Catalysis, Transition-Metal Reactivity by Design”, Girona, April 2018
- Main Organizer “*Progress in Theoretical Chemistry: Biomolecules and Materials*” Symposium at XXXVI Reunión Bienal RSEQ, Sitges, June 2017
- Main Organizer Girona Seminar 2016: “Predictive Catalysis, Transition-Metal Reactivity by Design”, Girona, April 2016
- Organizer XXXI Meeting Catalan Research Network (XRQTC), June 2015, Girona
- Main Organizer First scientific workshop COST Action CM1305 (ECOSTBio), Sept. 2014, Girona
- Main Organizer CECAM/ESF workshop on “Spin states in biochemistry and inorganic chemistry”, Zaragoza (Sept. 2012, www.cecarn.org/workshop-671.html); highlighted in *Nature Chem.* 2013, 5, 7-9
- “Course on DFT/ADF” for *International Intensive Course* of European Master in Theoretical Chemistry and Computational Modelling, Madrid (ES), 2013; Groningen (NL), 2015
- Leader ADF workshop (invited) in Riviera Maya (MX), 2011 and Barcelona (ES), 2008
- Member of local organizing committee of Girona Seminars 2006, 2008, 2010 and 2012

Commissions of trust

- Member Steering Committee Catalan Research Network XRQTC (2016-)
- Member University Council (*Consell de Govern*) Univ. Girona (2015-)
- Member University Committee for Research, Technology Transfer and Doctorate Studies (*Comissió Delegada de Recerca, Transferència i Doctorat del Consell de Govern*), University of Girona (2015-)
- Member of *Comité de Usuarios de la Red Española de Supercomputación* (CURES) (2014-)
- Member *Claustre Univ. Girona* (controlling supervisory body) (2012-)

Referee and evaluation committees

- Member evaluation committees *Agencia Nacional de Evaluación y Prospectiva* (ANEP) for postdoctoral scholarships (Spring 2011, Spring 2014) and short-term research visits (Autumn 2011)
- Member of PhD tribunals/reading committees in Amsterdam (2008, 2011), Barcelona (2009, 2014, 2016, 2016), Girona (2011), Groningen (2015, 2016, 2017), Leiden (2006), Madrid (2017), Perugia (2017), Tarragona (2011, 2013), Uppsala (2015)
- Referee for >30 international scientific journals (total reports since Sep. 2009: >500)
- Referee for funding agencies (NWO, FWO, ANEP, SARA, SNF, PRACE)

Editorial boards scientific journals and Editor of books and journals

- Associate Editor *RSC Advances* (Oct. 2015-Oct. 2016)
- Editor of Wiley Book (release date Nov. 2015) on *Spin states in biochemistry and inorganic chemistry*
- Member of Editorial Board of *Journal of Computational Methods in Science and Engineering* (2006-now), *Computational Chemistry Highlights* (2012-now), *Journal of Serbian Chemical Society* (2014-now), *Journal of Molecular Graphics and Modelling* (2015-now), *Inorganica Chimica Acta* (2016-now)
- Guest Editor for *Current Inorganic Chemistry* (2012) and *Current Organic Chemistry* (2013)

Referee for following international scientific journals

Acc. Chem. Res. – Centr. Eur. J. Chem. – Chem. Commun. – Chem. Eur. J. – ChemPhysChem – Chem. Phys. Lett. – Chem. Sci. – Comput. Theor. Chem. – Coord. Chem. Rev. – Dalton Trans. – Eur. J. Inorg. Chem. – Inorg. Chem. – Inorg. Chim. Acta – Int. J. Quant. Chem. – J. Am. Chem. Soc. – J. Biomol. Struct. Dyn. – J. Chem. Inf. Model. – J. Chem. Theory Comput. – J. Comput. Chem. – J. Inorg. Bioch. – J. Mol. Graph. Model. – J. Mol. Model. – J. Organomet. Chem. – J. Phys. Chem. A/B/C – J. Phys. Chem. Lett. – Mol. Phys. – Mol. Simulat. – Monatsh. Chem. – Nature Chem. – New. J. Chem. – Org. Biomol. Chem. – Organometallics – Phys. Chem. Chem. Phys. – Phys. Status Solidi – PLOS One – RSC Advances – SoftMatter – Theochem – Theor. Chem. Acc.

Total number of reviews (since Sep. 2009): >500

Plenary speaker at internationally established conferences

- *International Congress of Quantum Chemistry (ICQC16)*, Menton (FR), 2018
- *PAC Symposium*, Utrecht (NL), 2017
- *VII Current Trends in Theoretical Chemistry conference*, Kraków (PL), 2016
- *Annual meeting of the Serbian Chemical Society*, Belgrade (RS), 2016

Keynote speaker at internationally established conferences

- *FemEx 2017*, Huizen (NL), 2017
- *Netherlands Conference on Chemistry and Catalysis (NCCC)*, Noordwijkerhout (NL), 2017
- *9th European Biological Inorganic Chemistry (Eurobic) conference*, Wroclaw (PL), 2008

Invited presentations (based on invitation letter) to internationally established conferences (since 2008)

- *Japan-France-Spain symposium on theoretical chemistry for complex systems*, Kyoto (JP), 2016
- *CECAM Workshop: Modeling activity vs. selectivity in metalloproteins*, Paris (FR), 2015
- *Final meeting of COST Action CM1003*, Lisbon (PT), 2015
- *XIth Girona seminar on Carbon/Metal-Carbon Clusters*, Girona (ES), 2014
- *DFT-based Multilayer Methods for Nanoscale Systems workshop*, Leiden (NL), 2013
- *4th Georgian Bay Intl. Conference on Biological Inorganic Chemistry (CanBic)*, Toronto (CAN), 2013
- *ICQC Satellite UCLA*, Los Angeles, 2012
- *TEDxUdG*, Girona (ES), 2012
- *XXXVII Congreso de Químicos Teóricos de Expresión Latina (Quitel)*, Riviera Maya (MX), 2011
- *XXXIII Reunión Bienal de la Real Sociedad Española de Química*, Valencia (ES), 2011
- *IXth Girona seminar on Electron Density, Density Matrices, Density Functional Theory*, Girona (ES), 2010
- *Intl. Conference on Computational Methods in Science and Engineering (ICCMSE '09)*, Rhodes (GR), 2009

Invited presentations (based on selected abstract) to internationally established conferences (since 2008)

- *251st National Meeting of the ACS*, San Diego (USA), 2016
- *Pacificchem 2015*, Honolulu (USA), 2015
- *16th International Conference on Density Functional Theory*, Debrecen (HU), 2015
- *Annual meeting of the French BioInorganic Chemistry group (FrenchBIC)*, Anglet (FR), 2014
- *Second Society Meeting of Chemical Biology Group of RSEQ*, Bilbao (ES), 2014
- *First International Workshop on Protein Electron Transfer*, Modena (IT), 2013
- *15th International Conference on Density Functional Theory*, Durham (UK), 2013
- *16th International Conference on BioInorganic Chemistry (ICBIC16)*, Grenoble (FR), 2013
- *13th International conference on Density Functional Theory*, Lyon (FR), 2009
- *MGMS Spring Meeting on Bioinorganic Chemistry*, Cardiff (UK), 2008
- *37th Inorganic Reaction Mechanisms Group Meetings*, Barcelona (ES), 2008

Invited presentations at research centers (since 2008)

KTH Royal Institute of Technology Stockholm (2016) – VU Univ. Amsterdam (2015) – Univ. Groningen (2015) – Univ. Delft (2015) – Univ. Groningen (2014) – Univ. Uppsala (2013) – Univ. Dublin (2013) – Techn. Univ. Berlin (2013) – ICIQ, Tarragona (2012) – IQTCUB, Barcelona (2012) – Houk group, UCLA (2012) – Univ. Belgrade (2012) – Univ. Tromsø (2011) – BSC Life Sciences, Barcelona (2011) – Univ. Rochester (NY) (2008)

Membership of scientific societies

- Fellow, Royal Society of Chemistry (2015-)
- Member, American Chemical Society (2015-)
- Member, Young Academy of Europe (2014-)
- Member, Society of Biological Inorganic Chemistry (2010-)
- Member, Real Sociedad Española de Química (2009-)
- Member, Societat Catalana de Química (2008-)
- Member, Research Network “Xarxa de Referència en Química Teòrica i Computacional” (2006-)

Outreach activities

- External expert (“Meet the boss”) on “External economic affairs: Europe and the outer world”, *Erasmian European Youth Parliament Girona 2017*, INS Santiago Sobrequés (high-school, Girona), Feb. 2017
- Visit to INS Santiago Sobrequés (high-school, Girona), *Dia de la ciencia en primera persona 2016* program, “I’m a Chemist..... (Sóc Químic)”. Nov. 2016
- Visit to INS Salvador Espriu (high-school, Girona), *Dia de la ciencia en primera persona 2015* program, “I’m a Chemist..... (Sóc Químic)”. Nov. 2015
- Introductory lecture at *Matins de Química 2014* (Univ. Girona, Chemistry Dept.), “I’m a Chemist..... (Sóc Químic)”, Jan. 2014, www.goo.gl/1DK88F
- Visit to CRP Alt Empordà (high-school, Girona), *Dia de la ciencia a les escoles 2013* program, “I’m a Chemist..... (Sóc Químic)”. Nov. 2013, www.goo.gl/q6wAEu
- Host at Fira de la Ciència de Secundària (visit by high-school students), May 2013, www.goo.gl/HID3Yy
- Invited popular science paper in *Anales de Química*, “Regioselectividad en fullerenos, una visión computacional”, *An. Quím.* **2013**, 109, 11-19, www.goo.gl/ev4Pi2
- Visit to INS Vilablareix (high-school, Girona), *La ciencia en primera persona* program, “I’m a Chemist..... (Sóc Químic)”. Plus interview by high-school students (www.goo.gl/b8376t), Nov. 2012
- Talk at TEDxUdG, “I’m a Chemist.....”, May 2012, <http://youtu.be/YRegn8WnSdg>
- Member of CatQuimica.Cat team, blog (in Catalan) created for International Year of Chemistry (2011)

Authorship established software

- Co-author of the following computational chemistry software: ADF program, NWChem program
- Main author of the following computational chemistry software: DRF90, pdb2adf, QUILD

Other achievements

- Elected Director of *Institut de Química Computacional i Catalisi* (IQCC) (July 2015-July 2019)
- Invited presentations: >40 (since 2008), >60 (all years), <http://www.marcelswart.eu/agenda/index.html>
- Research stays at Univ. Belgrade (2012, 2013, 2016), UCLA (2012), Univ. Guanajuato (2011)
- Member of *Comissió Permanent* (G8) of the Institute of Computational Chemistry and Catalysis (2013-)
- Elected member of the *Claustre* of Universitat de Girona (2012-2016), the official body of the University that has a controlling function and has to approve annually the activities of the Rector
- Session leader at XI Girona Seminar, Girona, 2014; Multiscale Modelling conference, Manchester, 2014; XXVIII Reunió de la XRQTC, Barcelona, 2012; X Girona Seminar, Girona, 2012; MGMS Bioinorganic Chemistry meeting, Cardiff, 2008
- Organizer DFT popularity poll (DFT2010-DFT2015), www.marcelswart.eu/dft-poll
- Invited speaker on seminar tour in Japan: Yokohama, Osaka, Sendai, Tokyo, (2003)

Personal information

<i>Name</i>	Marcel Swart
<i>Title</i>	Dr. (PhD), defense 10 September 2002 Prof. (ICREA Research Professor) FRSC (Fellow of the Royal Society of Chemistry) FYAE (Fellow of the Young Academy of Europe)
<i>Citizenship</i>	Dutch
<i>Gender</i>	Male
<i>Marital status</i>	Married
<i>Office address</i>	<u>ICREA Research Professor at</u> Institut de Química Computacional i Catalisi & Departament de Química Universitat de Girona Campus Montilivi (Ciències) c/ Maria Aurèlia Capmany, 69 17003 Girona, Spain
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