

# Curriculum Vitae

Marcel Swart

Professor Dr. FYAE FRSC MAE

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## 1 Personal details

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## 2 Appointments

07/2015 – present Director of IQCC Institute, University of Girona  
09/2009 – present ICREA Professor at 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 received from *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 20 contributed talks and over 30 posters at national and international conferences

(selected Invited \* / Keynote \*\* / Plenary \*\*\* talks; <sup>M</sup> major conferences; <sup>r</sup> rescheduled<sup>COVID19</sup>)

- xx/2024** \*<sup>rM</sup> 15th European Biologic Inorganic Chemistry conference (EuroBic), Reykjavik (IS)  
**08/2022** \*<sup>rM</sup> 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 \* 35<sup>th</sup> Winter School in Theoretical Chemistry 2019: Inorganic Chemistry, Helsinki (FI)  
**08/2019** \*<sup>M</sup> 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 \* 11<sup>th</sup> Congress on Electronic Structure and Principle (ESPA2018), Toledo (ES)  
07/2018 \* International Conference on Porphyrins and Phthalocyanins (ICPP10), Munich (DE)  
**06/2018** \*<sup>M</sup> 16<sup>th</sup> International Conference on Quantum Chemistry (ICQC), Menton (FR)  
04/2018 \* Annual meeting EuroDoc, Tampere (FI)  
11/2017 \* Workshop "Missions of Universities over Time: Global Actors, National Champions  
or Local Power Houses?", Stockholm (SE)  
11/2017 \* DFT2017: Development and Application of Density Functional Theory, Lyon (FR)  
**08/2017** \*<sup>M</sup> 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 \*\*\* 53<sup>rd</sup> Annual meeting of Serbian Chemical Society, Kragujevac (RS)  
05/2013 \* 4<sup>th</sup> International Conference on Biological Inorganic Chemistry (CANBIC-4), Parry  
Sound (CAN)  
05/2012 \* TEDxUdG, Girona (ES)  
12/2011 \* XXXVII Congreso de Químicos Teóricos de Expresión Latina (Quitel), Riviera Maya  
(MX)  
**09/2008** \*\*<sup>M</sup> 9<sup>th</sup> European Biological Inorganic Chemistry (EuroBic) conference, Wroclaw (PL)

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

Indian Institute of Technology (IIT) Roorkee (2021<sup>online</sup>) – LMU Munich (2021<sup>online</sup>) – Univ. Oxford  
(2020<sup>online</sup>) – Univ. Sheffield (2020<sup>online</sup>) – 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 activities

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)
01/2018	Panel member ALLEA Workshop “Ethical aspects of Open Access: A Windy Road”, 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)
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:

- H2020 HPC-Europa3 visits by Eoin O'Sullivan (Oxford) and Robert Gericke (Trinity), 2021
- MCIN R&D Project "CorrFunc", 121.000€ + PhD fellowship (PI), 2021-2024
- MCIN R&D Support Funding for European proposals "FuncDens", 10.000€ (PI), 2019-2021
- UdG Project Promotors2019 IQCC, 60.000€ (PI as Director IQCC), 2020-2022
- RES Supercomputing Projects (2.148.480h), 2021-2022
- Beatriu de Pinós V. Elumalai, 144.300€ (PI), 2021-2024
- MINECO PhD Fellowship F. Martins, 92.750€ (PI), 2019-2023
- Consolidated group QTMEM, 0€ (Co-I), 2017-2021
- Unlimited site license ADF program package (developer, SCM), 2002-present

Furthermore, I'm collaborator in H2020-SWAFS project of the YAE ([www.caliper-project.eu](http://www.caliper-project.eu)), H2020-FetOpen project FRINGE, and NSF (I. Garcia-Bosch) projects, with other proposals (including those of collaborators) currently under evaluation.

Previously funded grants include 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).

## 8 Supervision, expert evaluations and examination panels

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 part of the FWO Evaluation Panel for Chemistry (Flanders), and form(ed) part of 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, and expert for evaluations of research proposals of ANEP, AvH, DFG, Fondecyt, FWO, FWF, GACR, LaCaixa, MSCA, NSC Poland, NWO, PRACE, Royal Society, SARA, SNF.

I have been member of promotion panels of staff at UCSD (2016), IOCB (2018), Trinity (2019), and Tromsø (2021).

## 9 Selected administrative duties and committee work

09/2021 – 11/2021	Member of Scientific Committee TAM meeting (HPC Europa3)
10/2019 – present	Member of Advisory Council of Young Academy of Europe
09/2019 – present	Member of UdG Steering Committee for HRS4R
06/2019 – present	Member of UdG committee for Communication
04/2018 – present	Founding Member and Vice-President Quantum-BioInorganic Chemistry (QBIC) Society
04/2018 – present	Founding Member and Vice-President <i>Grupo Especializado Química y Computación</i> (GEQC) of Spanish Chemical Society (RSEQ)
05/2017 – present	Member Higher Education, Research and Culture in European Societies (HERCuES) group
03/2012 – present	Member of UdG Claustre (equivalent to Senate)
11/2018 – 10/2019	Outgoing Chair Young Academy of Europe
03/2018 – 09/2019	External Scientific Advisory Board, Foster Plus, <a href="http://www.fosteropenscience.eu">www.fosteropenscience.eu</a>
01/2018 – 09/2020	Member of UdG committees for Quality Control, International Policy
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
03/2016 – 07/2020	Member Management Board, Catalanian Research Network XRQTC
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
04/2014 – 09/2019	Member of <i>Comité de Usuarios de la Red Española de Supercomputación</i>

## 10 Academic leadership

Selected Conference, Seminar, and Colloquium organisation:

06/2010 – present	Annual DFT Popularity Poll, see guest post on guest post on Nature Chemistry's Sceptical Chymist blog, <a href="https://bit.ly/5yearsDFTPoll">https://bit.ly/5yearsDFTPoll</a>
04/2018	Girona Seminar on Predictive Catalysis: Transition-Metal Reactivity by Design (gender-balanced invited speaker list; presence of Prof B Feringa, Nobel Laureate Chemistry 2016); 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)
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)
09/2012	CECAM/ESF Workshop on "Spin states in biochemistry and inorganic chemistry", highlighted in Nature Chem. 2013, 5, 7-9 (Zaragoza, ES)

## 11 Teaching

I have been engaged with different forms of teaching ranging from tutoring secondary-school scholars, to lecturing Erasmus, Bachelor, Master, PhD students and postgrads. ICREA Professors are not expected to teach, and an additional contract from the UdG is required (achieved in 2017). I have taught at the European Master in Theoretical Chemistry (2013, 2015), ECOSTBio Training Schools (2015, 2016), and since 2018 teach regularly at the UdG for undergrad, Master and PhD students to great satisfaction of the students. Topics are quantum chemistry, Density Functional Theory, biomolecular design, science communication and Open Science.

## 12 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).

## 13 Editorial responsibilities

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>
02/2006 – present	Member Editorial Board <i>Journal of Computational Methods in Science and Engineering</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)
06/2013	Guest editor special issue <i>Current Organic Chemistry</i> on "Nanoreactors And Molecular Prisons"
06/2012	Guest editor special issue <i>Current Inorganic Chemistry</i> on "Chameleon-like behavior of transition-metal complexes"
Reviewer activity	See: <a href="https://publons.com/a/1212468/">https://publons.com/a/1212468/</a> and <a href="http://www.bit.ly/MSwartORCID">www.bit.ly/MSwartORCID</a>