

Curriculum Vitae

Professor Dr. Marcel Swart FYAE FRSC

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1 Personal details

IQCC Institute, Department of Chemistry
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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, 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

09/2017 Special award in honour of 120 years anniversary of Serbian Chemical Society
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; ^M major conferences)

- 06/2020 * 11th International Conference on Porphyrins and Phthalocyanines (ICPP11), Buffalo (NY) (USA)
- 08/2019 *^M** 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 *^M** 16th 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 *^M** 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)
- 05/2012 * TEDxUdG, Girona (ES)
- 12/2011 * XXXVII Congreso de Químicos Teóricos de Expresión Latina (Quitel), Riviera Maya (MX)
- 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):

Univ. Oxford (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

01/2018	Panel member ALLEA Workshop “Ethical aspects of Open Access: A Windy Road”, Brussels (BE)
10/2017	<i>Panel member SAPEA Workshop, Tallinn (EE) (cancelled because of 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 over 3m EUR for science, outreach and equipment from the Spanish and Catalan Governments, the European Union (FP7, H2020) and Industry. The type of grants includes COST Action, Marie Curie Fellowships x2, Juan de la Cierva Fellowships x2, Europa Excelencia, and *Proyectos de Excelencia I+D* (including associated PhD fellowships).

8 Supervision, teaching, and examining

I have been engaged with different forms of teaching ranging from tutoring secondary-school scholars, to lecturing 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 part of the FWO Evaluation Panel for Chemistry (Flanders), and formed part of LaCaixa panel for PhD fellowships, Spanish national evaluation agency (ANEP) for postdoctoral fellowships and short-term visits of staff members. I am member of the BSC/RES Users Committee, and expert for evaluations of research proposals of ANEP, DFG, FWO, FWF, GACR, NWO, PRACE, Royal Society, SARA, SNF.

9 Selected administrative duties and committee work

11/2018 – 10/2019	Outgoing Chair Young Academy of Europe
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)
03/2018 – present	External Scientific Advisory Board, Foster Plus, www.fosteropenscience.eu
01/2018 – present	Member of UdG committee for Quality Control
05/2017 – present	Member Higher Education, Research and Culture in European Societies (HERCuLES) group
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 – present	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 – present	Member of <i>Comité de Usuarios de la Red Española de Supercomputación</i> (CURES)
03/2012 – 03/2014	Member of UdG Committee for Doctoral Programme in Chemistry
03/2012 – present	Member of UdG Claustre

10 Academic leadership

Selected Conference, Seminar, and Colloquium organisation:

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)
06/2010 – present	Annual DFT Popularity Poll, see guest post on Nature Chemistry's Sceptical Chymist blog, https://goo.gl/tDSk7L

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 Editorial responsibilities

03/2016 – present	Member Editorial Board <i>Inorganica Chimica Acta</i>
10/2015 – 10/2016	Associate Editor <i>RSC Advances</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>
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)
03/2013 – 09/2015	Member Editorial Board <i>Frontiers in Chemistry: Theoretical and Computational Chemistry</i>
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"
02/2006 – present	Member Editorial Board <i>Journal of Computational Methods in Science and Engineering</i>
Reviewer activity	See: https://publons.com/a/1212468/