

CARMEN DOMENE-NÚÑEZ

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Department of Chemistry
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Nationality: Spanish/British



EDUCATION

- 2012 – 2014 PGCAP, King's College London
Higher Education Research Network Journal runner up prize
- 01/98 – 12/00 PhD in Chemistry, University of Exeter
Thesis title: Many-body effects in interionic interactions. Supervisor: Prof P. W. Fowler
Lovis Rydon Memorial Research Prize
- 1996 – 1997 PGCE in Sciences, Instituto de Ciencias de la Educación, University of Seville (Spain)
First Class with distinction
- 1995 – 1997 Postgraduate Courses in Physical Chemistry, Department of Chemistry, University of Seville (Spain)
First Class with distinction
- 1990 – 1995 MSc in Chemistry, University of Seville (Spain) Five-year Degree

PROFESSIONAL EXPERIENCE

- 2017-Present Professor of Computational Chemistry, University of Bath, Department of Chemistry
- 2012-2023 Academic Visitor, University of Oxford, Department of Chemistry
- 2012-2017 Reader in Computational Chemistry, King's College London, Department of Chemistry
- 2003- 2011 Royal Society University Research Fellow, University of Oxford, Department of Chemistry
- 2001-2003 PDRA, University of Oxford, Laboratory of Molecular Biophysics, Department of Biochemistry

VISITING POSITIONS

- 2021-2022 Harvard University, Department of Molecular and Cellular Biology (USA), Gaudet group
- 2017 University of Brasilia, Cellular Biology Department (Brazil)
- 2010-2011 University of Maryland, School of Pharmacy, Baltimore (USA), Mackerell group
- 2010 The Institute of Mathematics, Chennai (India), Vemparala group
Institut Laue-Langevin, Grenoble (France), Wacklin's guest
- 2009 National Institute of Advanced Industrial Science & Technology, Tsukuba, (Japan), Shinoda group
Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, (Italy), Laio group
- 2005-2008 ETH Zurich, Department of Chemistry and Applied Biosciences (Switzerland), Parrinello group
EMBO fellowship awardee and Royal Society international project exchange
- 2005 Uppsala University, Department of Cell and Molecular Biology (Sweden), Aqvist group
J. W. T. Jones Fellowship, Royal Society of Chemistry
- 2004-2006 University of Pennsylvania, Laboratory for Research on the Structure of Matter (USA), Klein group

PUBLICATIONS Summary

>120 publications in internationally refereed journals (see Appendix)

<http://scholar.google.co.uk/citations?user=VvGQZCwAAAAJ&hl=en>

Researcher unique identifiers: Research ID: A-2711-2019; ORCID ID: 0000-0001-7115-4232; Scopus ID: 7004155411

Prizes & AWARDS

- 2023 Royal Society of Chemistry Corday-Morgan Prize
- 2020 International Society of Quantum Biology and Pharmacology (ISQBP) Loew award
- 2014 Higher Education Research Network Journal Prize, runner up
- 2006 EMBO short-term fellowship
- 2005 J.W.T. Jones Fellowship, Royal Society of Chemistry
- 2003-2011 Royal Society University Research Fellowship, The Royal Society of London
- 1999 Lovis Rydon Memorial Research Prize (for best thesis work)
- 1997 Formación del Personal Investigator Fellowship, Junta de Andalucía (Spain)

PROFESSIONAL SERVICE

- Fellow of the Royal Society of Chemistry (2016)
- Elected Member, Council Royal Society of Chemistry (2015-2018), (2019-2022)
- Nominations Committee, Royal Society of Chemistry (2019-2022)
- EPSRC College member (2006-2012), (2016-2023)
- STFC E-Infrastructure Advisory Group (2021-2024)
- European Science Foundation College of reviewers (2016-2023)
- The International Society of Quantum Biology and Pharmacology (ISQBC), Council (2016-2024)
- Royal Society International Conference Grants and Short Visits Committee, Panel 3 (2007-2009)
- Royal Society Research Grants, Board B (2009-2018)
- Member of the Resource Allocation Panel (RAP) for the National HPC Service (2013-2016)
- PRACE (Partnership for Advanced Computing in Europe) user forum programme committee (2016-2022)
- The Royal Society of Chemistry (Faraday Division), Travel and Scientific Meetings Grants Committee (2016-2019)
- The Royal Society of Chemistry, RSC's Researcher Mobility Grant Working Group (2018-2021)
- Spanish Researchers in the UK (SRUK-CERU), Travel and Scientific Meetings Grants Committee (2014-present)
- Biophysical Society Committee member, Professional Opportunities for Women Committee (2013-2019)
- Biophysical Society Committee member, Membership Committee (2020-2023)
- Member of the Royal Society of Chemistry (2000), the American Chemical Society (2010), Biophysical Society (2002), Spanish Researchers in the UK (SRUK-CERU) (2012), Spanish Biophysical Society (2014), the International Society of Quantum Biology and Pharmacology (2015), Spanish Royal Society of Chemistry (2018).
- Member of National & International Review Panels:
 - 2006-2012, 2016-2023 Engineering and Physical Sciences Research Council (EPSRC) UK
 - 2008 Research Frontiers Programme of Science Foundation (SFI) Ireland
 - 2017 Fundação para a Ciência e a Tecnologia (FCT) Portugal, Bioengineering and Biotechnology panel
 - 2019 H2020-FETOPEN European Commission Research Executive Agency
 - National Science Centre (NSC), Poland, Expert Panel 'Molecular biology, structural biology, biotechnology'
 - 2020 H2020-FETOPEN European Commission Research Executive Agency
 - Fundação para a Ciência e a Tecnologia (FCT) Portugal, Bioengineering and Biotechnology panel
 - Deutsche Forschungsgemeinschaft Germany
 - Spanish National Agency for Scientific Evaluation (ANEP), Juan de la Cierva Fellowships Panel
 - 2021 National Science Centre (NSC), Poland, Expert Panel 'Molecular biology, structural biology, biotechnology'
 - HORIZON-EIC-PATHFINDEROPEN European Innovation Council & SMEs Executive Agency
 - Fundação para a Ciência e a Tecnologia (FCT) Portugal, Chemistry panel
 - Georgian National Science Foundation
 - 2022 UKRI-STFC CoSeC Impact Award (CIA)
 - National Science Centre (NSC), Poland, Expert Panel 'Molecular biology, structural biology, biotechnology'
 - British-Spanish Society, SRUK/CERU Emerging Talent Award 2022 (Chair)
 - Fundação para a Ciência e a Tecnologia (FCT) Portugal, Chemistry panel (Co-chair)
 - IntDisRP Interdisciplinary Expert Panel, Research Foundation Flanders
 - Georgian National Science Foundation
 - HORIZON-MSCA-PF-2022
 - EuroHPC
 - HORIZON-EIC-PATHFINDEROPEN European Innovation Council & SMEs Executive Agency
 - European Research Council
 - 2023 UKRI-STFC CoSeC Impact Award (CIA) (Chair)
 - Fundação para a Ciência e a Tecnologia (FCT) Portugal, Chemistry panel
 - IntDisRP Interdisciplinary Expert Panel, Research Foundation Flanders (Belgium)
 - EuroHPC
 - HORIZON-EIC-PATHFINDEROPEN European Innovation Council & SMEs Executive Agency
 - European Research Council
 - Postdoctoral Junior Leaders "la Caixa" Fellowship Programme (Spain)
 - Georgian National Science Foundation

Estonian National Science Foundation
Slovenian National Science Foundation

- Book Reviewer for the Royal Society of Chemistry & Oxford University Press.
- COST Actions, UK delegate: [1] CM1103, (2011-2015) MC Member; [2] CM1207 GLISTEN (2013-2017) MC Substitute; [3] CA21160 COZYME (2022-2026) MC Member, [4] CA21162 ML4NGP (2022-2026) MC Member
- **Editorial Activities:** The Open Structural Biology Journal (2007-2010), Computational and Mathematical Methods in Medicine (2010-2013), Biophysical Journal (2010-2016), Open Biophysical Journal (2012-2015), BioMed Research International (2013-2021), Computational Biology (2013-2015), Frontiers: Biological Modelling and Simulation (2019-2023), Advisory Committee Soft Matter RSC (2019-2023), Molecular Physics (2022-).

MEETING ORGANIZATION

- 2010 Royal Society International Scientific Seminars - Kavli Seminars. Chicheley, UK
Coarse-Grained Modelling of Biological Systems (Organiser)
- 2014 Royal Society International Scientific Seminars, Indo-UK Seminars, Chennai (India) (Organiser).
- 2014 Royal Society of Chemistry (Faraday Division) Recent Appointees in Physical Chemistry, East Anglia (Organiser)
- 2014 Biophysical Society Annual Meeting, San Francisco, USA (Session Organiser)
- 2014-17 SRUK Annual Symposium, London UK (Organising Committee)
- 2018 CECAM meeting on 'Frontiers in Computational Biophysics: understanding conformational dynamics of complex lipid mixtures relevant to biology' (PI and Organiser). Lugano (Switzerland).
- 2018 CECAM meeting on 'Multiscale modelling in electrophysiology: from atoms to organs' (PI and Organiser). Lugano (Switzerland).
- 2018 Symposium on 'Computer Simulation in the Physical & Life Sciences', Rome (Italy).
- 2020 CECAM meeting on 'Ions, membrane and channels: Multiscale simulations from quantum to coarse-grain; a symposium in honour of Mike Klein's 80th birthday'. Paris (France)
- 2022 'MolSim22: Computer Simulation: From Materials to Chemical Biology'. Erice (Italy)

List of Selected Publications (2019-2023)

Research Papers

- 23** N-aryltetrahydroisoquinoline derivatives as HA-CD44 interaction inhibitors: design, synthesis, computational studies, and antitumor effect.
J.M. Espejo-Román, B. Rubio-Ruiz, M. Chayah-Ghaddab, C. Vega-Gutierrez, G. García-García, A. Muguruza-Montero, C. Domene, R.M. Sánchez-Martín, O. Cruz-López, A. Conejo-García
Eur. J. Med. Chem. **2023**, 258, 115570-83.
- 22** Redox regulation of KV7 channels through EF3 hand of calmodulin.
E. Nuñez, F. Jones, A. Muguruza-Montero, J. Urrutia, A. Aguado, C. Malo, G. Bernardo-Seisdedos, C. Domene, O. Millet, N. Gamper, A. Villarroel
Elife **2023**, 12, e81961.
- 21** Early Steps in C-type Inactivation of the hERG Potassium Channel
F. Pettini, C. Domene, S. Furini
J. Chem. Inf. Model. **2022**, 63 (1), 251-258.
- 20** Selective anticancer therapy based on a HA-CD44 interaction inhibitor loaded on polymeric nanoparticles.
J. M. Espejo-Román, B. Rubio-Ruiz, V. Cano-Cortés, O. Cruz-López, S. Gonzalez-Resines, C. Domene, A. Conejo-García, R. M. Sánchez-Martín
Pharmaceutics **2022**, 14(4), 788.
- 19** A potential route of capsaicin to its binding site in the TRPV1 ion channel.
C. Domene, L. Darre, V. Oakes, S. Gonzalez-Resines
J. Chem. Inf. Model. **2022**, 62, 10, 2481-2489.
- 18** An integrated mass spectrometry and MD simulations approach reveals the spatial organization impact of metal-binding sites on the stability of metal-depleted metallothionein-2 species.
M. D. Peris-Díaz, R. Guran, C. Domene, V. Rios, O. Zitka, V. Adam, A. Krężel
J. Am. Chem. Soc. **2021**, 143 (40), 16486-16501.
- 17** Ion conduction mechanism is a fingerprint of potassium channels.
C. Domene, R. Ocello, M. Masetti, S. Furini

- J. Am. Chem. Soc.* **2021**, 143 (31), 12181-12193.
- 16 Multiple interactions of glucose with the extramembraneous loops of GLUT1 aid transport.
S Gonzalez-Resines, P J Quinn, R J Naftalin, C Domene
J. Chem. Theory Comput. **2021**, 61 (7), 3559-3570.
- 15 The ligand-bound state of a G protein-coupled receptor stabilizes the interaction of functional cholesterol molecules.
L. Lemel, K. Nieścierowicz, M. Busnelli, L. Darré, M.D. Garcia Fernandez, M. Pezet, B. Mouillac, M. Vivaudou, C. Domene, B. Chini, V. Cherezov, C.J. Moreau
J. Lipid Res. **2021**, 62, 100059.
- 14 KATP channel with a DEND syndrome mutation induces hyperpolarization in murine skeletal muscle.
S. Horita, T. Ono, S. Gonzalez-Resines, Y. O. M. Yamachi, S. Zhao, C. Domene, Y. Maejima, K. Shimomura
Sci. Rep. **2021**, 11(1), 6668.
- 13 Conduction and gating properties of the TRAAK channel from molecular dynamics simulations with different force fields.
R. Ocello, S. Furini, F. Lugli, M. Recanatini, C. Domene, M. Masetti
J. Chem. Inf. Model. **2020**, 60, 12, 6532–6543.
- 12 Differential stability of Aurein 1.2 pores in model membranes of CIDCA133 and CIDCA331 probiotics strains.
G.E. Balatti, C. Domene, M.F. Martini and M. Pickholz
J. Chem. Inf. Model. **2020**, 60 (10), 5142-5152.
- 11 Effect of anionic lipids on ion permeation through the KcsA K⁺-channels.
V. Oakes, S. Furini, C. Domene
BBA-Biomembranes, **2020**, 1862 (11), 183406.
- 10 Affinity for the interface underpins potency of antibodies operating in membrane environments.
E. Rujas, S. Insausti, D. P. Leaman, P. Carravilla, S. Gonzalez-Resines, V. Monceaux, R. Sanchez-Eugenia, M. Garcia-Porras, I. Iloro, L. Zhang, F. Elortza, J-P. Julien, A. Saez-Cirion, M. B. Zwick, C. Eggeling, A. Ojida, C. Domene, J. M.M. Caaveiro, J. L. Nieva.
Cell Reports, **2020**, 32 (7), 108037.
- 9 Critical assessment of common force fields for Molecular Dynamics simulations of potassium channels.
S. Furini, C. Domene
J. Chem. Theory Comput. **2020**, 16 (11), 7148-7159.
- 8 Mechanism of oxygen diffusion in a model oxygenase through multiscale simulation.
C. Domene, C. Jorgensen, C.J. Schofield
J. Am. Chem. Soc. **2020**, 142(5), 2253-2263.
- 7 The bilayer collective properties govern the interaction of an HIV-1 antibody with the viral membrane.
P. Carravilla, I. Ruiz-Oar, E. Rujas, L. Darre, C. Domene, J.L. Nieva, J. Requejo-Isidro
Biophys J **2020**, 118 (1), 44-56.
- 6 Insights into the mechanisms of K⁺ permeation in K⁺-channels from computer simulations.
V. Oakes, S. Furini, C. Domene
J. Chem. Theory Comput. **2020**, 16(1), 794-799.
- 5 Influence of cholesterol and its stereoisomers on members of the serotonin receptor family.
V. Oakes, C. Domene
J. Mol. Biol. **2019**, 431 (8), 1633-1649.
- 4 Antibiotic resistance and host immune evasion in *Staphylococcus aureus* mediated by a novel metabolic adaptation.
J-H Jiang, M. S. Bhuiyan, H.-H. Shen, D. R. Cameron, T. Rupasinghe, C.-M. Wu, X Kostoulas, C. Domene, A. J. Fulcher, M. J. McConville, B P. Howden, G. J. Lieschke and A. Y. Peleg
Proc. Natl. Acad. Sci. U.S.A., **2019**, 116 (9), 3722-3727.
- 3 Modulation of the KcsA potassium channel by anionic phospholipids: Role of the non-annular arginines.
J.A. Poveda, A.M. Giudici, M.L. Renart, O. Millet, A. Morales, J.M. González-Ros, V. Oakes, S. Furini, C. Domene
BBA-Biomembranes, **2019**, 183029.
- 2 Investigating the mechanism of action of anesthetics using computer simulation.
V. Oakes and C. Domene
Chem. Rev. **2019**, 119 (9), 5998-6014.

- 1 Combining Structural Data with Computational Methodologies to Investigate Structure–Function Relationships in TRP Channels
V. Oakes, C. Domene
TRP Channels: Methods and Protocols, **2019**, 65-82.

Selected Invited Talks (2019-2023)

- Instituto de Física de Buenos Aires (IFIBA), Universidad de Buenos Aires (Argentina) Dec 2023
- XLVI Congreso Internacional de Químicos Teóricos de Expresión Latina, Montevideo (Uruguay) Nov 2023
- The University of São Paulo, School of Medicine, Ribeirão Preto (Brazil) Nov 2023
- Center for Bioinformatics and Integrative Biology (CBIB), Universidad Andres Bello, Santiago (Chile) Oct 2023
- "Frontiers in ion channels and nanopores", Rome (Italy), Sep 2023
- Center for Bioinformatics and Integrative Biology (CBIB), Universidad Andres Bello, Santiago (Chile) Nov 2022
- Department of Chemistry, Cardiff University, Cardiff (UK), Oct 2022
- Institute of Neuroscience, Spanish Council for Scientific Research, Alicante, (Spain) Sep 2022
- InfraLife, Integrative Structural Biology Summer School, Stockholm (Sweden) Sep 2022
- EMBO workshop 'Membrane transporters as essential elements of cellular functions and homeostasis' Chania (Greece), 28 Aug–1 Sep 2022
- The President's Meeting 2022, Int Society of Quantum Biology and Pharmacology, Innsbruck (Austria), Jul 2022
- Center for Bioinformatics and Integrative Biology (CBIB), Universidad Andres Bello, Santiago (Chile) Dec 2021
- TrEnCa, Trends in Enzyme Catalysis, Castellon (Spain), Dec 2021
- 72nd Annual Meeting of the International Society of Electrochemistry, Jeju Island, Korea, 29 Aug – 3 Sept 2021
- American Chemical Society Fall Meeting 2021, Atlanta (USA) Aug 2021
- The President's Meeting 2020, Int Society of Quantum Biology and Pharmacology, Strasburg (France), Jun 2021
- AMO seminar committee, Department of Physics and Astronomy, University of Delaware (USA), Mar 2021
- Center for Bioinformatics and Integrative Biology (CBIB), Universidad Andres Bello, Santiago (Chile) Dec 2020
- Centro Nacional de Biotecnología, CSIC, Madrid (Spain), Apr 2020
- Department of Chemistry, University of Nottingham (UK), Jan 2020
- Telluride workshop on 'Ion Channel Biophysics', Telluride (USA), Jul 2019
- Joint 12th EBSA 10th ICBP - IUPAP Biophysics Congress, Madrid (Spain) Jul 2019
- 11th International Conference on Chemical Kinetics, Orleans (France) Jun 2019
- Milestones in Molecular Simulations with Prof Parrinello, London (UK) Jun 2019
- XXXVII Chemistry Biennial 2019 Spanish Royal Society of Chemistry, San Sebastian (Spain) May 2019
- 6th ECBS/LS-EuChemS meeting, Madrid (Spain) Apr 2019
- 'Molecular Dynamics Today' workshop, University of Bologna, Bologna (Italy) Mar 2019
- Department of Chemistry, University of Vienna, Vienna (Austria) Feb 2019
- Department of Biochemistry, University of Bristol, Bristol (UK) Jan 2019