W. M. C. SAMEERA

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PROFILE

Accomplished materials science researcher with a strong foundation in computational modelling and data-driven approaches. I hold a PhD (plus postdoctoral or equivalent experience) in computational materials science, combining domain expertise with automated discovery of novel materials. I have a proven record of securing external research funding (national, European, industrial) and leading multi-partner projects. I supervise and mentor students (BSc, MSc, PhD) and contribute to high-impact publications. My technical expertise includes advanced materials modelling (*ab initio* and ML-accelerated methods), proficiency in programming, and experience in experimental integration. I am collaborative, proactive, and enthusiastic about bridging computational and experimental techniques to foster scientific breakthroughs.

EDUCATION AND RESEARCH TRAINING

2009 - 2010: Postdoctoral Research Fellow, University of Oxford. United Kingdom.
2006 - 2009: Ph.D. (computational chemistry), University of Glasgow, United Kingdom.
2001 - 2006: B.Sc. (Hons.) in Chemistry, University of Sri Jayewardenepura, Sri Lanka.

PROFESSIONAL PROFILE

2025 : Researcher, Department of Space, Earth and Environment, Chalmers University of Technology, Sweden.
2016 - 2024: Assistant Professor, Institute of Low Temperature Science, Hokkaido University, Japan.
2014 - 2016: Japan Society for the Promotion of Science (JSPS) fellowship, Fukui Institute for Fundamental Chemistry, Kyoto University, Japan.
2013 - 2014: Marie Curie ITN fellowship, University of Gothenburg, Sweden.
2010 - 2012: Research Fellow, Institute of Chemical Research of Catalonia, Spain.

FELLOWSHIPS & PRIZES

2024 Professorship (visiting), The Fellows in Residence program, CY Cergy Paris Université, France.
2023 Associate Professorship (visiting), Institute for Chemical Research, Kyoto University, Japan.
2022 Senior Lecturer (visiting), Department of Chemistry, University of Colombo, Sri Lanka.
2022 Visiting Scholar, CY Cergy Paris Université, France.
2017 Visiting Scholar, Department of Chemistry and Molecular Biology, University of Gothenburg, Sweden.
2016 Visiting Scholar, Department of Chemistry, University of Kelaniya, Colombo, Sri Lanka.
2014 Japan Society for the Promotion of Science (JSPS) fellowship, Fukui Institute for Fundamental Chemistry, Kyoto University, Japan.
2013 Marie Curie ITN fellowship, University of Gothenburg, Sweden.
2011 Best poster prize, World Association of Theoretical and Computational Chemists 2011, Spain.
2011 Postdoctoral fellow, Institute of Chemical Research of Catalonia, Spain.
2010 Postdoctoral fellow (EPSRC), Inorganic Chemistry Laboratory, University of Oxford, United Kingdom.
2009 Best poster prize, the seventh Canadian Computational Chemistry Conference, Canada.
2008 Jim Gatheral Scholarship, University of Glasgow, United Kingdom.
2006 WestCHEM postgraduate fellowship, School of Chemistry, University of Glasgow, United Kingdom.

TEACHING

- 2021 – 2023: Quantum Chemistry, BSc fourth year students (14 students).
- 2021 – 2023: Computer programming in Chemistry, BSc fourth year students (10 students).
- 2021 – 2023: Quantum Chemistry, BSc third year students (40 students).
- 2021 – 2023: Inorganic Spectroscopic Methods, BSc third year students (40 students).
- 2021 – 2023: Computational Chemistry Practical Classes BSc third- or fourth-year students (10 students)

- 2021 – 2023: Analytical Chemistry, MSc students (40 students)
- 2016 – 2019: Coordination Chemistry, BSc first year students (10 students).
- 2018 – 2020: Visiting lectures in Computational Chemistry (20 students).

UNIVERSITY PEDAGOGY TRAININGS AND WORKSHOPS

- 2025: Teaching and Learning in Higher Education, University of Gothenburg, Sweden.
- 2022: Workshops on Teaching in Higher Education, University of Colombo.
- 2018: Workshops on innovative pedagogies, Hokkaido University.

SUPERVISION

Undergraduate students (BSc):

- **2024 – 2025: Kristoffer Hansson** (Supervisor)
- **2024 – 2025: Heesara Lokuhapuarachchi** (Supervisor)
- 2024 – 2025: Pathum Sandaruwan (Supervisor) // (Now a PhD student t Penn State University, USA)
- 2023 – 2024: Pabasara Ediriweera (Supervisor) // (Now a PhD student at University of Arizona, USA)
- 2023 – 2024: Pansidu Weraharage (Supervisor) // (Now a PhD student at Wayne State University, USA)
- 2022 – 2023: Ashini. N. de Silva (Supervisor) // (Now a PhD student at Virginia Tech, USA).
- 2022 – 2023: Charith Kuruppu // (Moving to the University of Florida, USA)
- 2022 – 2023: Lakshan Weerasinghe (Supervisor) // (Now a PhD student at Ohio State University, USA).
- 2022 – 2023: Nimasha Thejani (Supervisor) // (Now a PhD student at Northeastern University, USA).
- 2023 – 2024: Shalith Chamantha (Supervisor) // (Now a PhD student at Iowa State University, USA).
- 2022 – 2023: Danushi Pathirage (Now a PhD student at the University of Nebraska, USA).

MSc students:

- 2024 – 2025: Lasith Tharanga (Supervisor) // (Now a PhD student at Stony Brook University, USA)
- 2024 – 2025: Piumali Sanjeewani. (Supervisor) // (Now a PhD student at Louisiana State University, USA).
- 2023 – 2024: Waruna Hashan (Supervisor) // (Now working in industry).
- 2023 – 2024: Chathura Senarathne (Supervisor) // (Now a PhD student at Queen's University in Canada).
- 2022 – 2023: Thilini Geekiyanage (Supervisor) // (Now working in industry).
- 2017 – 2019: Sae Yanagida (Co-supervisor) // (Now working in industry).
- 2017 – 2019: Ayao Watanabe (Co-supervisor) // (Now working in industry).
- 2017 – 2019: Chuei Akasugi (Co-supervisor) // (Now working in industry).

PhD students:

- **2025 – 2029: Satsuki Nomura** (Co-supervisor)
- **2024 – 2028: Hema Malani** (Co-supervisor)
- 2017 – 2020: Tomo Ogawa (Co-supervisor) // (Now an Assistant Professor, Kyushu University)
- 2017 – 2020: Panyi Liang (Co-supervisor) // (Now a postdoctoral fellow at SUSTech, China)

Postdoctoral researchers:

- 2015 – 2017: Akhilesh K. Sharma (Co-supervisor) // (Now a postdoctoral fellow at Institute of Chemical Research of Catalonia).
- 2015 – 2017: Miho Isegawa (Co-supervisor) // (Now a postdoctoral fellow at Kyushu University).

Visiting researchers:

- 2019: Yanying Zhao, Associate Professor, Zhejiang Sci-Tech University, China. (Supervisor)
- 2016: Victor Fernandez, Prof. Feliu Maseras Group, Institute of Chemical Research of Catalonia. (Supervisor)
- 2014. Fernando Castro, Prof. Calers Bo Group, Institute of Chemical Research of Catalonia. (Supervisor)
- 2014. Divya Sharma, Prof. Martin Paterson Group, Heriot-Watt University, UK. (Supervisor)

GRANTS

Current grants

1) 2024-2026: The Fellows in Residence program, CY Cergy Paris Université, France.
   Interstellar chemical evolution: roles of OH anion-driven reactivity. (**Principal Investigator**)
2) 2025-2028: Japan Society for the Promotion of Science KAKENHI grant. (No. 25H00677)
   https://kaken.nii.ac.jp/grant/KAKENHI-PROJECT-25H00677/
   Synthesis of nucleic acid and its precursors from extraterrestrial organic molecules in primordial Earth environments. ***(Co-Investigator)***
3) 2020-2026: International Collaborative Research Program of Institute for Chemical Research, Kyoto University.

N_2 reduction $Cp^{XL}{}_3Mo_3S_4M$ clusters (M = Fe, Ni, Co): an ab-initio computational study. (**Principal Investigator**)

4) 2022-2027: Japan Society for the Promotion of Science KAKENHI grant (No. 22H00159). https://kaken.nii.ac.jp/en/grant/KAKENHI-PROJECT-22H00159/
Molecular evolution on the surface of interstellar dust activated by radical diffusion: the key to the production of complex organic molecules. (**Co-Investigator**)

Previous grants

5) 2023-2024: Grant from the Japan Science and Technology Agency Sakura Science Program.
This grant funded seven chemistry students in the Department of Chemistry, University of Colombo, Sri Lanka to visit the Institute for Chemical Research at Kyoto University in Japan for a research stay. (**Principal Investigator**)
6) 2022-2024: Japan Society for the Promotion of Science Bilateral Joint Research Project grant (No. JPJSBP 120229901).
Predicting radical behaviours on interstellar dust surface: a collaborative theoretical and experimental approach. (**Principal Investigator**)
7) 2022-2023: CY Advanced Studies, CY Cergy Paris Université, France.
Connect computational chemistry, surface science, and low-temperature sciences to study the radical processes on ice. (**Principal Investigator**)
8) 2021-2023: Japan Society for the Promotion of Science KAKENHI grant (No. 21H05416) https://kaken.nii.ac.jp/en/grant/KAKENHI-PUBLICLY-21H05416/
Quantum chemical determination of the complex organic molecules' formation in the interstellar medium. (**Principal Investigator**)
9) 2019-2021: Japan Society for the Promotion of Science KAKENHI grant (No. 19K03940). https://kaken.nii.ac.jp/en/grant/KAKENHI-PROJECT-19K03940/
Multiscale modelling of radical diffusion and radical reactions on interstellar ices. (**Principal Investigator**)
10) 2017-2021: Japan Society for the Promotion of Science KAKENHI grant (No. 17H06445). https://kaken.nii.ac.jp/en/grant/KAKENHI-PLANNED-17H06445/
Elucidation of mechanism for hybrid catalytic systems based on the automated reaction path search method. (**Co-Investigator**)
11) 2014-2016: Japan Society for the Promotion of Science grant (No. P14334).
Computational study of the reaction mechanism and selectivity of synthetic chiral metalloporphyrins. (**Principal Investigator**)

PUBLICATIONS

2025

1) K. Hansson, W. M. C. Sameera,* J. C. Esmerian, D. Bossion, S. Andersson, S. Aalto, W. Vlemmings, K. K. Knudsen, G. Nyman. ***Astron. Astrophys.*** 2025 (Accepted) https://arxiv.org/abs/2508.19339
2) T. J. L. C.Bakx, L. Sommovigo, Y. Tamura, R- Smit, A. Ferrara, H. Algera, S. Aalto, D. Bossion, S. Carniani, C. Esmerian, M. Hagimoto , T. Hashimoto, B. Hatsukade, E. Ibar, H. Inami, A. K. Inoue, K. Knudsen, N. Laporte, K. Mawatari, J. Molina, G. Nyman, T. Okamoto, A. Pallottini, W. M. C. Sameera, H. Umehata, N. Yoshida, ***Mon. Not. R. Astron. Soc.*** 2025, 544, 1502-513.
3) T. Higaki, K. Tanaka, S. Oishi, H. Izu, K. Kawamoto, M. Tada, W. M. C. Sameera, R. Takahata, T. Teranishi, S. Kikkawa, S. Yamazoe, T. Shiga, M. Nihei, T. Kato, R. E. Cramer, Z. Zhang, K. Meyer, Y. Ohki. ***J. Am. Chem. Soc.*** 2025, 147, 3215-3222.
4) B. Corbin, P. Ediriweera, C. Salmon, K. M. Arachchige, Yi. Pang, W. M. C. Sameera, C. S. Abeywickrama. ***J. Phys. Chem. B***, 2025, 129, 19, 4189-4203.
5) Y. Matsuoka, Y. Sakai, H. Izu, M. Fujisawa, M. Tada, N. M. Lakshan, W. M. C. Sameera, K. Tanifuji, Y. Ohki, ***Coordination Chemistry Research***, 2025, 1, 100001.

2024

6) S. Kondo, N. Yoshimura, A. Kobayashi, K. D. C. Kuruppu, W. M. C. Sameera, M. Yoshida, M. Kato. ***J. Mater. Chem. C***, 2024, 12, 1799-1808.
7) T. Nguyen, Y. Oba, W. M. C. Sameera, K. Furuya, N. Watanabe. ***Astrophys. J.*** 2024, 976, 250.
8) T. Saito, M. Yoshida, K. Segawa, D. Saito, J. Takayama, S. Hiura, A. Murayama, N. M. Lakshan, W. M. C. Sameera, A. Kobayashi, M. Kato. ***Chem. Sci.*** 2024, 15, 14497-14505.
9) A. P. Jayaweera, B. Senevirathne, S. Weerasighe, N. Watanabe, G. Nyman, F. Dulieu, W. M. C. Sameera,****ACS Earth Space Chem***. 2024. 8, 1451-1459.

10) Y. Matsuoka, Y. Sakai, H. Izu, M. Fujisawa, M. Tada, N. M. Lakshan, W. M. C. Sameera, K. Tanifuji, ***Coordination Chemistry Research***, 2024, 1, 100001.
11) **REVIEW:** N. M. Lakshan, D. C. Aluthge, W. M. C. Sameera,* ***Catalysts***, 2024, 14, 816.
12) **BOOK CHAPTER:** W. M. C. Sameera, Y. Sumiya, B. B. Skjelstad, S. Maeda, Automated mechanism discovery, ***Comprehensive Computational Chemistry***, 2024, 4, 454-484.
13) A. Ishibashi, H. Hidaka, W. M. C. Sameera, Y. Oba, N. Watanabe, ***Astrophys. J.*** 2024, 960, 90.
14) R. Kandler, Y. Benaragama, M. Bera, C. Wang, R. A. Samiha, W. M. C. Sameera, S. Das, A. Nag, ***Molecules***, 2024, 29, 2148.

2023

15) H. Izu, D. G. Bhave, Y. Matsuoka, W. M. C. Sameera,* K. Tanifuji, Y. Ohki, ***Eur. J. Inorg. Chem.*** 2023, 26, e202300399.
16) N. Balucani, M. Bertin, M. Brann, W. A. Brown, C. Ceccarelli, R. Martın-Domenech, J. Fulker, R. T. Garrod, J. Green, M. S. Gudipati, D. E. Heard, E. Herbst, U. Jacovella, I. Kamp, M. R. S. McCoustra, W. M. C. Sameera, I. Sims, A. Sturm, S. Viti, S. W. Weaver, L. Wiesenfeld, O. H. Wilkins, ***Faraday Discuss.*** 2023, 245, 519-540.
17) W. M. C. Sameera,* A. P. Jayaweera, A. Ishibashi, H. Hidaka, Y. Oba, N. Watanabe, ***Faraday Discuss.*** 2023, 245, 508-518.
18) Y. Nakai, W. M. C. Sameera, K. Furuya, H. Hidaka, A. Ishibashi, N. Watanabe, ***Astrophys. J.*** 2023. 953, 162.
19) T. Nguyen, Y. Oba, W. M. C. Sameera, K. Furuya, A. Kouchi, N. Watanabe. ***Astrophys. J.*** 2023, 944, 146.

2022

20) Ohki, Y. Munakata, R. Hara, M. Kachi, K. Uchida, M. Tada, R. E. Cramer, W. M. C. Sameera, T. Takayama, Y. Sakai, S. Kuriyama, Y. Nishibayashi, K. Tanifuji, ***Nature***, 2022, 607, 86-90.
21) T. Darshani, S. R. Samarakoon, F. R. Fronczek, W. M. C. Sameera, I. C. Perera, T. Perera, ***Bioinorg Chem Appl.*** 2022. DOI: https://www.hindawi.com/journals/bca/2022/7821284/
22) N. Vitharana, C. Kaushalya, T. Perera, S. Deraniyagala, W. M. C. Sameera, A. Cooray. ***ACS Omega***, 2022, 7, 32, 28342-28350.
23) K. Tanifuji, Y. Sakai, Y. Matsuoka, M. Tada, W. M. C. Sameera, Y. Ohki, ***Bull. Chem. Soc. Jpn.*** 2022, 95, 1190-1195.
24) **BOOK CHAPTER:** W. M. C. Sameera,* Y. Takeda, Y. Ohki. ***Advances in Organometallic Chemistry***, 2022, 78, 35-78.
25) **REVIEW:** W. M. C. Sameera,* B. Senevirathne, T. Nguyen, Y. Oba, A. Ishibashi, M. Tsuge, H. Hidaka, N. Watanabe, ***Front. Astron. Space Sci.*** 2022, 9, 890161.

2021

26) T. Nguyen, Y. Oba, W. M. C. Sameera, A. Kouchi, N. Watanabe, ***Astrophys. J.*** 2021, 922, 146.
27) T. Fujita, M. Yamane, W. M. C. Sameera, H. Mitsunuma, M. Kanai, ***Angew. Chem. Int. Ed.*** 2021, 60, 24598-24604.
28) T. Nguyen, Y. Oba, W. M. C. Sameera, A. Kouchi, N. Watanabe, ***Astrophys. J.*** 2021. 198, 73.
29) N. Thushara, T. Darshani, S. R. Samarakoon, I. C. Perera, F. R. Fronczek, W. M. C. Sameera, T. Perera. ***RSC. Adv.*** 2021,11, 17658-17668.
30) Y. Takeda, K. Toyoda, W. M. C. Sameera,* N. Tohnaia, S. Minakata, ***Adv. Synth. Catal.*** 2021, 363, 2796-2805.
31) J. Stenger-Smith, I. Chakraborty, R. Ouattara, W. M. C. Sameera, K. Rue, P. Mascharak. ***Chem. Commun.*** 2021, 57, 1101-1104.
32) K. Kitajima, Y. Nakai, W. M. C. Sameera, M. Tsuge, A. Miyazaki, H. Hidaka, A. Kouchi, N. Watanabe. ***J. Phys. Chem. Lett.*** 2021, 12, 1, 704-710.
33) W. M. C. Sameera,* B. Senevirathne, S. Andersson, M. Al-Ibadi, H. Hidaka, A. Kouchi, G. Nyman, N. Watanabe. ***J. Phy. Chem. A***, 2021, 125, 1, 387-393.

2020

34) A. Miyazaki, N. Watanabe, W. M. C. Sameera, Y. Nakai, M. Tsuge, T. Hama, H. Hidaka, A. Kouchi. ***Phys. Rev. Lett. A***, 2020, 102, 052822.
35) **REVIEW:** Y. Takeda, W. M. C. Sameera,* S. Minakata, ***Acc. Chem. Res.*** 2020, 53, 1686-1702.
36) Y. Ohki, K. Ishihara, M. Yaoi, M. Tada, W. M. C. Sameera, R. E. Cramerd, ***Chem. Commun.*** 2020, 26, 9537-9546.
37) K. Ishihara, Y. Araki, M. Tada, T. Takayama, Y. Sakai, W. M. C. Sameera,* Y. Ohki, ***Chem. Eur. J.*** 2020, 26, 9537-9546.
38) C. Wakasugi, M. Yoshida, W. M. C. Sameera, Y. Shigeta, A. Kobayashi, M. Kato, ***Chem. Eur. J.*** 2020, 26, 5449-5458.
39) T. Ogawa, W. M. C. Sameera, M. Yoshida, A. Kobayashi, M. Kato, ***Chem. Phys. Lett.*** 2020, 137024.

2019

40) N. Watanabe, W. M. C. Sameera, H. Hidaka, A. Miyazaki, A. Kouchi, ***Chem. Phys. Lett.*** 2019, 737, 136820.
41) J. González-Fabra, F. Castro-Gómez, W. M. C. Sameera, G. Nyman, A. Kleij, C. Bo, ***Catal. Sci. Technol.*** 2019, 9, 5433-5440.
42) S. Yanagida, M. Yoshida, W. M. C. Sameera, A. Kobayashi, M. Kato, Masako, ***Bull. Chem. Soc. Jpn.*** 2019, 92, 1684-1693.
43) Y. Takeda, T. Matsuno, A. K. Sharma, W. M. C. Sameera,* S. Minakata, ***Chem. Eur. J.*** 2019, 25, 10226-10231.

44) M. Yoshida, H, Shitama, W. M. C. Sameera, A. Kobayashi, M. Kato, ***Chem. Eur. J.*** 2019, 25, 7669-7678.
45) A. K. Sharma, W. M. C. Sameera,* Y. Takeda, S. Minakata. ***ACS Catal.*** 2019, 9, 4582-4592.

2018

46) T. Ogawa, W. M. C. Sameera, M. Yoshida, A. Kobayashi, M. Kato, ***Inorg. Chem.*** 2018, 57, 14086-14096.
47) Y. Ohki, K. Uchida, R. Hara, M. Kachi, M. Fujisawa, M. Tada, Y. Sakai, W. M. C. Sameera, ***Chem. Eur. J.*** 2018, 24, 17138-17147.
48) W. M. C. Sameera,* F. Maseras, ***J. Chem. Info. Model.*** 2018, 58, 1828-1835.
49) A. Olmos, R. Gava, B. Noverges, D. Bellezza, M. Besora, W. M. C. Sameera, M. Etienne, F. Maseras, G. Asensio, A. Caballero, P. J. Pérez, ***Angew. Chem. Int. Ed.*** 2018, 57, 13848-13852.
50) P. Liang, A. Kobayashi, W. M. C. Sameera, M. Yoshida, M. Kato, ***Inorg. Chem.*** 2018, 57, 5929-5938.
51) **BOOK CHAPTER:** R. Ramozzi, W. M. C. Sameera, K. Morokuma, Predicting reaction pathways from reactants, *Applied Theoretical Chemistry*, PP. 321-349, Ed. Dean J. Tantillo, World scientific publishing. (ISBN: 978-1-78634-408-3)
52) T. Ogawa, W. M. C. Sameera, M. Yoshida, A. Kobayashi, M. Kato, ***Dalton Trans.*** 2018, 47, 5589-5594.
53) J. Jimenez, I. Chakraborty, A. Dominguez, J. Martinez-Gonzalez, W. M. C. Sameera, P. K. Mascharak, ***Inorg. Chem.*** 2018, 57, 1766-1773.
54) J. Stenger-Smith, I. Chakraborty, W. M. C. Sameera, P. K. Mascharak, ***Inorg. Chim. Acta.*** 2018, 471, 326-335.

2017

55) J. Stenger-Smith, I. Chakraborty, W. M. C. Sameera, P. K. Mascharak, ***Inorg. Chim. Acta***. 2018, 471, 326-335. 2017.
56) A. K. Sharma, W. M. C. Sameera, M. Jin, Masayoshi, L. Adak, C. Chiemi, T. Iwamoto, M. Kato, M. Nakamura, K. Morokuma, ***J. Am. Chem. Soc.*** 2017, 16117-16125.
57) M. Isegawa, W. M. C. Sameera, A. K. Sharma, T. Kitanosono, M. Kato, S. Kobayashi, K. Morokuma, ***ACS Catal.*** 2017, 7, 5370-5380.
58) W. M. C. Sameera,* B. Senevirathne, S. Andersson, F. Maseras, G. Nyman, ***J. Phy. Chem. C***, 2017, 121, 15223-15232.
59) **BOOK CHAPTER:** B. Jayawardena, D. Pandithavidana, W. M. C. Sameera,* Polysaccharides in solution: experimental and computational studies. *Solubility of Polysaccharides*, Ed. Zhenbo Xu (ISBN: 978-953-51-5443-3)
60) M.-C. Yang, A. K. Sharma, W. M. C. Sameera, K. Morokuma, M.-D. Su, ***J. Phys. Chem. A***, 2017, 121, 2665-2673.
61) I. Chakraborty, J. Jimenez, W. M. C. Sameera, M. Kato, P. K. Mascharak, ***Inorg. Chem.*** 2017, 56, 2863-2873.
62) A. Watanabe,a A. Kobayashi, E. Saito, Y. Nagao, S. Omagari, T. Nakanishi, Y. Hasegawa, W. M. C. Sameera, M. Yoshida, M. Kato, ***Inorg. Chem.*** 2017, 56, 3005-3013.
63) L. Maestre, R. Dorel, O. Pablo, I. Escofet, W. M. C. Sameera, E. Álvarez, F. Maseras, M. M. Diaz-Requejo, A. M. Echavarren, P. J. Pérez, ***J. Am. Chem. Soc.*** 2017, 139, 2216-2223.

2016

64) Y. Ohki, Y. Shimizu, R. Araake, M. Tada, W. M. C. Sameera, J.-I. Ito, H. Nishiyama, ***Angew. Chem. Int. Ed.*** 2016, 128, 16053-16057.
65) D. Sharma, W. M. C Sameera, S. Andersson, G. Nyman, M. J. Paterson, ***ChemPhysChem***, 2016, 17, 4079-4089.
66) S. Inaba, W. M. C. Sameera, *J. Phys. Chem. A*, 2016, 120, 6670-6676.
67) **REVIEW:** W. M. C. Sameera, A. K. Sharma, S. Maeda, K. Morokuma, ***Chem. Rec.*** 16, 2016, 2349-2363.
68) Y. Takeda, A. Kuroda, W. M. C. Sameera, K. Morokuma, S. Minakata, ***Chem. Sci.*** 2016, 7, 6141-6152.
69) S. Sasaki, S. Suzuki, W. M. C. Sameera, K. Igawa, K. Morokuma, G. Konishi, ***J. Am. Chem. Soc.*** 2016, 138, 8194-8206.
70) **REVIEW:** W. M. C. Sameera, S. Maeda, K. Morokuma, ***Acc. Chem. Res.*** 2016, 49, 763-773.
71) I. Funes-Ardoiz, W. M. C. Sameera, R. M. Romero, C. Martínez, J. A. Souto, D. Sampedro, K. Muñiz, F. Maseras, ***Chem. Eur. J.*** 2016, 22, 7545-7553.

2015

72) W. M. C. Sameera, M. Hatanaka, T. Kitanosono, S. Kobayashi, K. Morokuma, ***J. Am. Chem. Soc.*** 2015, 137, 11085-11094.
73) REVIEW: L. W. Chung, W. M. C. Sameera, R. Ramozzi, A. J. Page, M. Hatanaka, G. P. Petrova, T. V. Harris, X. Li, Z. Ke, F. Liu, H-B. Li, L. Ding and K. Morokuma, ***Chem. Rev.*** 2015, 115, 5678-5796.
74) REVIEW: M. Besora, A. A. C. Braga, W. M. C. Sameera, J. Urbano, M. R. Fructos, P. J. Perez, F. Maseras, ***J. Organomet. Chem.*** 2015, 784, 2-12.

2014

75) J. Llaveria, Á. Beltrán, W. M. C. Sameera, A. Locati, M. M. Díaz-Requejo, M. I. Matheu, S. Castillón, F. Maseras, P. J. Pérez, ***J. Am. Chem. Soc.*** 2014, 136, 5342-5350.

76) E. M. Zueva, R. Herchel, S. Borshch, E. V. Govor, W. M. C. Sameera, R. McDonald, J. Singleton, Y. Sanakis, J. Krzystek, J. E. McGrady, R. G. Raptis, ***Dalton Trans***, 2014, 43, 11269-11276.

2013

77) L. Maestre, W. M. C. Sameera, M. M. Díaz-Requejo, F. Maseras, P. J. Pérez, ***J. Am. Chem. Soc***. 2013, 135, 1338-1348.
78) I. Rivilla, W. M. C. Sameera, E. Alvarez, M. M. Díaz-Requejo, F. Maseras, P. J. Pérez, ***Dalton Trans***, 2013, 42, 4132-4138.

2012 – 2008

79) V. P. Georgiev, W. M. C. Sameera, J. E. McGrady, ***J. Phys. Chem. C.*** 2012, 116, 20163-20172.
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RECENT TALKS (last six years)

2025

1) *Cosmic origins of catalysis: linking molecular evolution in space to sustainable chemistry on earth*, Institute for Chemical Research, Kyoto University, Japan. (Invited Lecture)
2) *From cosmic dust to molecules: computational approaches to rationalise interstellar chemical complexity*, Workshop on Computational Chemistry and Machine Learning for Chemical Physics, CY Cergy Paris Université, France. (Invited Lecture)
3) *On the reactivity of OH anions in interstellar ices*, CICO-VICO-CASSUM Spring 2025 Workshop, Gothenburg, Sweden. (Lecture)
4) *Quantum mechanical insights into the synthesis of complex organic molecules in cold interstellar environments*, Department of Space, Earth and Environment, Chalmers University of Technology, Sweden. (Lecture)

2024

5) *Atomic-scale modelling of chemical reactions*, Department of Biology, Edge Hill University, UK. (Lecture)
6) *Introduction to Quantum Chemistry*, Department of Chemistry, Sheffield Hallam University, UK (Lecture)

2023

7) *Multicomponent reactions on ice at low temperatures*, Sapporo-Colombo-Gothenburg Astrochemistry Meeting 2023, Gothenburg University, Sweden. (Lecture)
8) *Quantum chemical modelling of excited states and properties*, Kwansei Gakuin University, Japan. (Invited Lecture)
9) *OH radical on ice: photodesorption and reactivity from quantum chemical calculations*. Symposium on Next Generation Astrochemistry, Tokyo, Japan. (Lecture)
10) *Radical binding and radical reactions on interstellar ices: a combined experimental and quantum chemical study*, Asia Pacific Conference of Theoretical and Computational Chemistry, APATCC-10, Vietnam. (Invited Lecture)
11) *A systematic mechanistic survey on the reactions between OH radical and CH_3OH on ice*. Astrochemistry at high resolution Faraday Discussion. Maryland, United States. (Lecture)

2022

12) *Radical processes on interstellar ices: a combined experimental and quantum chemical study*. Symposium on Next Generation Astrochemistry, Japan. (Lecture)
13) *Quantum chemical modelling of the radical chemistry on ice surfaces*, Sapporo-Colombo-Gothenburg Astrochemistry meeting 2022, Gothenburg University, Sweden. (Lecture)

2021

14) *Quantum chemical determination of the complex organic molecules formation in the interstellar medium*, Next Generation Astrochemistry Symposium, Japan. (Lecture)
15) *Radical species on interstellar ices: a quantum chemical study*. The 15th annual meeting for Japan Society for Molecular Science 2021. (Lecture)

2020

16) *Radical species on interstellar ices: a quantum mechanics/molecular mechanics study*. CICO-VICO Fall 2020 Workshop, Chalmers University, Sweden. (Lecture)
17) *Advances and challenges in modelling reaction mechanisms*. Department of Chemistry School of Life Sciences, University of Sussex, UK. (Invited Lecture)
18) *On the mechanistic puzzles of homogeneous catalysis*. Institute for Materials Chemistry and Engineering, Kyushu University, Japan. (Invited Lecture)

2019

19) *Exploring mechanistic puzzles in Pd-catalysed aziridine ring-opening reactions*. The Asia-Pacific Association of Theoretical and Computational Chemists (APATCC), Sydney, Australia. (Invited Lecture)

2018

20) *Radical species on interstellar ices: some clues from a quantum mechanics/molecular mechanics study*. International workshop on interstellar matter 2018, Hokkaido University, Japan. (Invited Lecture)
21) *Palladium-catalysed regioselective and stereospecific ring-opening cross-coupling of 2-arylaziridines: computational studies*, University of Sydney, Australia. (Invited Lecture)
22) *Computational studies of Fe-catalysed C-C bond formation reactions*. The 43rd International Conference on Coordination Chemistry (ICCC 2018), Sendai, Japan. (Lecture)
23) *On the selectivity of the palladium-catalysed aziridine ring-opening reactions*, Fukui Institute for Fundamental Chemistry, Kyoto University, Japan. (Invited Lecture)
24) *A hybrid QM/MM approach to calculate binding energies of radical species on crystalline water ice*. Quantum Chemistry, Dynamics, and Reaction Modelling for Molecules and Materials in Astrophysical Environments, 255th National Meeting, New Orleans, LA, USA. (Invited Lecture)

2017

25) *On the mechanism and selectivity of transition metal-catalysed N-N and C-C bond formation reactions*. Asia pacific conference in theoretical and computational chemistry (APCTCC8), Mumbai, India. (Invited Lecture)
26) *On the selectivity of transition metal catalysis: DFT and MC-AFIR studies*, International conference on theoretical and high-performance computational chemistry 2017, Hangzhou, China. (Lecture)
27) *Computational studies on the catalytic and photophysical properties of transition metal complexes*, Department of Chemistry, Zhejiang Sci-Tech University, China. (Invited Lecture)
28) *Computational catalysis using quantum mechanics/molecular mechanics (QM/MM) and artificial force-induced reaction (AFIR) methods*, BIT's 8th Annual Global Congress of Catalysis 2017 (GCC-2017), Shanghai, China. (Invited Lecture)
29) *Systematic determination of complex reaction mechanisms. School of Physical and Mathematical Sciences*, Nanyang Technological University, Singapore. (Invited Lecture)
30) *Computational studies on the reactivity, selectivity, and photophysical properties of transition metal complexes*, University of Gothenburg, Sweden. (Invited Lecture)

ADMINISTRATIVE ROLES

- 2022-2025: Project manager, International Collaborative Research Program, Institute for Chemical Research, Kyoto University, Japan.
- 2023-2025: Project manager, Collaborative Research Program, CY Cergy Paris Université, France.
- 2022-2024: Coordinator, high-performance computing unit, University of Colombo.
- 2023-2024: Coordinator, computational chemistry program, Department of Chemistry, University of Colombo.
- 2023-2014: Student counsellor, Department of Chemistry, University of Colombo.
- 2016-2018: Developing curricula, evaluating international applicants, and the Integrated Science Program, Hokkaido University.
- 2016-2018: Member of the Integrated Science Program, Faculty of Science, Hokkaido University.

OUTREACH ACTIVITIES

- Conducted a hands-on workshop: Quantum chemical calculations, CY Cergy Paris Université, France. (2025)
  - This was a one-week workshop on quantum chemical calculations and machine learning.

- Established a student exchange program between Kyoto University in Japan and the University of Colombo in Sri Lanka. (2023)
- Organiser of the Sapporo-Colombo-Gothenburg Astrochemistry meeting 2023 and 2022, University of Gothenburg, Sweden.
- Conducted a hands-on workshop: Quantum chemical calculations, Kyoto University, Japan. (2023)
  - This was a one-week workshop for postgraduate students and postdoctoral researchers at the Institute for Chemical Research, Kyoto University.
- Conducted a hands-on workshop: Molecular docking, University of Sri Jayewardenepura, Sri Lanka. (2023)
  - This was a one-day workshop on applications of Molecular docking for biologists.
- Promoted English medium undergraduate courses of Hokkaido University. (2017)
  - Visited high schools and promoted undergraduate English-medium science courses at Hokkaido University.
- Conducted a hands-on workshop: Computational chemistry, University of Kelaniya, Sri Lanka. (2016)
  - This was a two-week workshop for final-year chemistry honours students, focusing on computational methods and applications.
- JSPS science dialogue program: The quantum mechanics of chemical reactions, Tokyo, Japan. (2016)
  - Visited high schools in Tokyo and delivered lectures on science.

INTERESTS

- Fluent in bass.