

CV

Personal information

Name: Dr. Dario Campisi

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Current institutional address: Institute for Theoretical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569, Stuttgart, Germany.

Education and Training:

14/09/2021 Ph.D. in Mathematics and Natural Sciences¹ (within MSCA-ITN EuroPAH), Leiden University, Leiden, the Netherlands, Thesis: "*Interstellar Catalysts and the PAH Universe*", Advisors: Prof. Dr. Alexander G. G. M. Tielens, Prof. Dr. Inge Loes ten Kate and Dr. Thanja Lamberts.

10/03/2017 MS.c. in Chemistry (grade 110/110), University of Palermo, Palermo, Italy, Thesis: "*Computational Study of the Catalytic Effects of Frustrated Lewis Pair Based Materials*", Advisors: Prof. Dr. Dario Duca and Dr. Remedios Cortese.

20/10/2014 BS.c. in Chemistry (grade: 92/110), University of Palermo, Palermo, Italy, Thesis: "*Optimization of Suzuki Reaction for the Synthesis of Derivatives of Interest in Optoelectronic*", Advisors: Prof. Dr. Michelangelo Gruttadauria and Prof. Dr. Francesco Giacalone.

Employment and Working Experiences

Present-1/10/2022 Head of Astrochemistry², Post-Doc, Humboldt fellow, University of Stuttgart, Stuttgart, Germany. Advisor: Prof. Dr. Johannes Kästner.

31/08/2022-1/10/2021 Postdoctoral Researcher, The University of Chicago, Chicago, USA, Advisor: Prof. Dr. Laura Gagliardi.

27/09/2021-30/08/2021 Postdoctoral Researcher³, Leiden University, Leiden, the Netherlands, Advisors: Prof. Dr. Alexander G. G. M. Tielens.

27/08/2021-28/08/2017 Early Stage Researcher⁴, Leiden University, Leiden, the Netherlands, funded by the Marie Skłodowska-Curie action (EuroPAH network), PI: Prof. Dr. Alexander G.G.M. Tielens.

- (3 Months) Secondment at Milan University, Milan, Italy. Project: "*Periodic DFT approaches: SIESTA code*", Advisor: Prof. Dr. Rocco Martinazzo.

- (1 Months) Secondment at Graphic Science, Bristol, UK. Project: "*Outreach Exhibition*", Advisor: Mr. Ben Johnson.

- (2 Months) Secondment at Aarhus University, Aarhus, Denmark. Project: "*Machine Learning Approaches*", Advisor: Prof. Dr. Bjørk Hammer

11/07/2017-11/03/2017 Voluntary Researcher, Computational Chemistry Center of Palermo (CCCP), Department of Physics and Chemistry, University of Palermo, Viale delle Scienze Parco d'Orléans II, Ed. 17, 90128 Palermo, Italy, Project: "*Hydrogenation and Dehydrogenation Processes by Metal-free BN Catalysts, using DFT Modeling*", Advisor: Prof. Dr. Dario Duca.

01/02/2013-01/11/2012 Pre-graduate Internship, National Research Council (CNR) - Institute for the Study of Nanostructured Materials 153, Via Ugo La Malfa, 90146 Palermo, Italy, www.ismn.cnr.it.

Project:

- *Multi-steps and one pot synthesis of materials (high surface area silica)*
- *Synthesis of hybrid organic-inorganic supported catalysts*

¹ The doctoral program in the Netherlands is 4 years and does not have a grade/rank.

² Fixed-term position. This is an internal project management position in the Kästner group.

³ Bridge contract of a month.

⁴ Position that implies research, training, secondments, outreach, teaching assistant.

Prizes, Awards, Grants, etc.

30/09/2024-1/10/2022 Humboldt Research Fellowship⁵ for Postdocs, University of Stuttgart, Stuttgart, Germany.
21/03/2022 Seal of Excellence for the Submitted Marie Curie Postdoctoral Fellowship proposal, 101064156- DFT-DMET-ML, Aarhus University.
22/08/2022-01/01/2018 Computational Time (~1400000 core hours) on HPC SurfSara (the Netherlands) and CINECA (Italy), *Granted Projects: EINF-154, EINF-1888, UARP, AFPP, IPCM, IPCM2, PFCM and APF*.
27/08/2020-28/08/2017 Marie Curie scholarship for PhD students (H2020 MSCA-ITN EuroPAH, grant number: 722346, PI: Prof. Dr. A.G.G.M. Tielens).

Referee Duties

08/09/2023-01/01/2022 Reviewer service for Astronomy & Astrophysics, J. Chem. Theory Comput., Chem. Mater., J. Phys. Chem, ACS Earth Space Chem. and Surf. Sci. journals.

Teaching Duties

31/07/2022-01/06/2022 Series of Lectures in Quantum Chemistry, The Gagliardi Group, The University of Chicago, Chicago, US. Lecturer: Dario Campisi
30/04/2021-30/01/2020 Modern Astronomical Physics Research and Modern Astronomical Research, Astronomy Bachelor's Course, Leiden University, Leiden, the Netherlands.
Teacher: Dr. Pedro Russo, Assistants: Dario Campisi, Stan Barmentloo and Ali Azadbakht.
27/11/2019 Astrochemistry, Liceo Scientifico Albert Einstein, Palermo, Italy, series of lectures to high school students. Lecturer: Dario Campisi
30/01/2020-2018 Astronomical Spectroscopy, Astronomy Master's Course, Leiden University, Leiden, the Netherlands. Teacher: Dr. Jordy Bouwman, Assistant: Dario Campisi.

Outreach Activities

27/04/2023 Girls Day⁶, University of Stuttgart, Stuttgart, Germany
18-27/07/2019 EUROPAH Astrochemistry pop-up shop⁷, The Galleries, Bristol, U.K..
19/11/2019 Astronomy on TAP, euroPAH⁸: "*A network of early-stage researchers*", Grand Cafe De Burcht, Burgsteeg 14, 2312 JS Leiden, the Netherlands.
29/09/2018 Explorathon⁹, Heriot-Watt University, Edinburgh, U.K..
27/08/2020-30/09/2017 Management of EuroPAH Public Blog¹⁰, <http://www.europah.com/>.

(Co-)organization of Scientific Meetings

1/09/2023-28/08/2023 Organizer¹¹ and Chair of the Mini-Symposium "*Surface Astrochemistry*" at the 36th, European Conference on Surface Science (ECOSS36), Lodz, Poland.
23-24/09/2019 SOC¹² PAHRTEA - *PAH Research: Theory, Experiments in an Astronomical context*; EUROPAH conference, Radboud University, Nijmegen, The Netherlands.

Institutional Responsibilities

28/08/2020-28/08/2018 Manager of the Interstellar Medium Group Meetings, Leiden Observatory, Leiden University, Leiden, the Netherlands.

(Co-)supervision of Students

31/10/2023-1/08/2022 Supervision of HIW¹³ student projects, Institute for Theoretical Chemistry, University of Stuttgart, Stuttgart, Germany. *Student: Annalena Riffelt and Severin Haid*.
31/05/2023-01/11/2022 Supervision of BSc Thesis Student Project¹⁴, Institute for Theoretical Chemistry, University of Stuttgart, Stuttgart, Germany. *Student: Annalena Riffelt*.¹⁵

⁵ Awarded through the Henriette Herz Scouting Programme for my research achievements.

⁶ Management of the astrochemistry section.

⁷ My role in this project was to team up with the other early-stage researchers to set up a scientific exhibition in which I took the direction of the quantum chemistry set-up.

⁸ Talk in a public space about the activities of EuroPAH network.

⁹ I teamed up with the other early-stage researchers for an open day exhibition in which I prepared a video and a poster about quantum chemistry and astrochemistry for people of all ages.

¹⁰ I wrote several blogs related to the EuroPAH activities and my research projects.

¹¹ My role was to prepare the conference schedule, invite speakers, evaluate the abstracts and chair the session.

¹² My role was to prepare the conference schedule, invite speakers and evaluate the abstracts.

¹³ A paid research internship student.

¹⁴ I have assigned the BSc project and being responsible for the outcome of the thesis and the graduation of the student.

¹⁵ Annalena was awarded 500 euros prize for an outstanding thesis by the industrial partner of the department of simulations and technologies.

01/08/2022-01/10/2021 Supervision of Postdoc Project¹⁶, **Chemistry Department, the University of Chicago, Chicago, US.** *Postdoc: Arup Sarkar.*

01/08/2022-01/02/2022 Supervision of Undergraduate Student Project¹⁷, Chemistry Department, the University of Chicago, Chicago, US. *Student: Manuela Pinheiro*

12/11/2021-01/09/2020 Supervision of Graduate Student Project¹⁸, Leiden Observatory, Leiden University, Leiden, the Netherlands. *Student: Morgan McCabe*

Computational Skills

Methods - Density Functional Theory, Coupled Cluster, Møller–Plesset Perturbation Theory, Surrogate Machine Learning potentials for QM (GPRs), QM/MM methods (ONIOM): Structural optimizations, Transition State search (Berni, NEB and Dimer methods). Transition State theory and Quantum Tunneling rate (Instanton, Square, Parabolic, Eckart, Wigner). Analysis of the electronic structure (DOS, PDOS, LDOS, COOP, COHP, population analysis). Isosurfaces, Harmonic vibrational frequencies and IR intensities. Counterpoise method (BSSE correction) and explicitly correlated F12 correction.

Codes - ORCA, GAUSSIAN, SIESTA, VASP, GPAW, Quantum Espresso, DFT-D4/D3. GOFEE and Catlearn (Machine Learning based on GPRs). kSC and DL-FIND/CHEMSHELL (tunnelling rate). METADISE (Interface and Surface preparation).

Programming - bash, python (mainly ASE and matlab).

Languages

Italian Mother tongue

English Fluent¹⁹

German Beginner

Publications

Peer-reviewed journal articles

1) D. Campisi²⁰, T. Lamberts, N. Y. Dzade, R. Martinazzo, I. L. ten Kate, A. G. G. M. Tielens, *Adsorption of Polycyclic Aromatic Hydrocarbons and C60 onto Forsterite: C–H Bond Activation by the Schottky Vacancy*, ACS Earth and Space Chemistry **2022**, 6, 8, 2009–2023. <https://doi.org/10.1021/acsearthspacechem.2c00084>

2) L. Wang, R. J. Papoular, N. E. Horwitz, J. Xie, A. Sarkar, D. Campisi²¹, N. Zhao, B. Cheng, G. L. Grocke, T. Ma, A. S. Filatov, L. Gagliardi, J. S. Anderson¹⁸, *Linker Redox Mediated Control of Morphology and Properties in Semiconducting Iron-Semiquinoid Coordination Polymers*, Angewandte Chemie International Edition **2022**, 61, e202207834; Angewandte Chemie **2022**, 134, e202207834. <https://doi.org/10.1002/anie.202207834>

3) A. M. Hastings, M. Fairley, M. C. Wasson, D. Campisi²¹, A. Sarkar, Z. C. Emory, K. Brunson, D. B. Fast, T. Islamoglu, M. Nyman, P. C. Burns, L. Gagliardi, O. K. Farha, A. E. Hixon, J. A. LaVerne¹⁸, *Role of Metal Selection in the Radiation Stability of Isostructural M–UiO-66 Metal–Organic Frameworks*, Chemistry of Materials **2022**, 34, 18, 8403–8417. <https://doi.org/10.1021/acs.chemmater.2c02170>

4) M. N. McCabe, P. Hemberger, D. Campisi²², J. C. Broxterman, E. Reusch, A. Bodi and J. Bouwman¹⁸, *Formation of phenylacetylene and benzocyclobutadiene in the ortho-benzyne + acetylene reaction*, Physical Chemistry Chemical Physics **2022**, 24, 1869–1876. <https://doi.org/10.1039/D1CP05183K>

5) D. Campisi²⁰, T. Lamberts, N. Y. Dzade, R. Martinazzo, I. L. ten Kate, A. G. G. M. Tielens, *Interaction of Aromatic Molecules with Forsterite: Accuracy of the Periodic DFT-D4 Method*, Journal of Physical Chemistry A **2021**, 125, 13, 2770–2781. <https://doi.org/10.1021/acs.jpca.1c02326>

6) R. Cortese, D. Campisi²³, A. Prestianni and D. Duca¹⁸, *Alkane Dehydrogenation on Defective BN Quasi-Molecular Nanoflakes: DFT Studies*, Molecular Catalysis **2020**, 493, 110891. <https://doi.org/10.1016/j.mcat.2020.110891>

¹⁶ Supervision of a postdoc's DFT calculations that resulted in a published article (<https://doi.org/10.1002/anie.202207834>)

¹⁷ Supervision of an Internship project.

¹⁸ Supervision of a PhD student's DFT calculations that resulted in a published article (<https://doi.org/10.1039/D1CP05183K>).

¹⁹ Certified at the University of Chicago Language Center.

²⁰ Corresponding author/Project leader.

²¹ I performed the theoretical calculations and wrote the theoretical part of the article.

²² I supervised M.N. McCabe's calculations and revised the theoretical part of the manuscript.

²³ I performed the theoretical calculations and revised the final draft of the manuscript.

7) **D. Campisi**²⁰ and A. Candian²⁰, *Do Defects in PAHs Promote Catalytic Activity in Space? Stone–Wales Pyrene as a Test Case*, *Physical Chemistry Chemical Physics* **2020**, 22, 6738–6748. <https://doi.org/10.1039/C9CP06523G>

8) **D. Campisi**²⁰, F. D. S. Simonsen, J. D. Thrower, R. Jaganathan, L. Hornekær, R. Martinazzo and A. G. G. M. Tielens, *Superhydrogenation of Pentacene: the Reactivity of Zigzag-Edges*, *Physical Chemistry Chemical Physics*, **2020**, 22, 1557–1565. <https://doi.org/10.1039/C9CP05440E>

9) R. Cortese, **D. Campisi**²³ and D. Duca²⁰, *Hydrogen Arrangements on Defective Quasi-Molecular BN Fragments*, *ACS omega*, **2019**, 4, 14849–14859. <https://doi.org/10.1021/acsomega.9b01445>

Others

10) **D. Campisi**²⁰, *Interstellar Catalysts and the PAH universe*, PhD thesis, **2021**, ISBN: 9789464192957. <https://hdl.handle.net/1887/3210124>

In preparation

11) **D. Campisi**²⁰, *Interstellar Grains Catalyze the Formation of Formamide 2023–2024*, in preparation

12) M.R. Schäfer and **D. Campisi**²⁰, *The Fragmentation of Naphthalene 2023–2024*, in preparation

14) S. Haid, K. Gugeler, J. Kästner, **D. Campisi**²⁰, *Super-Hydrogenation of Indene 2023–2024*, in preparation

15) F. Kruczkiewicz, B.M. Giuliano, **D. Campisi**²⁰, A. A. Gavdush, K. I. Zaytsev, G. A. Komandin, A. Ivlev, F. Ribeiro, P. Caselli¹⁸, *Far-Infrared Spectroscopy of Cryogenic N₂ and O₂ Molecular Solids at Low Pressure 2024*, in preparation

16) **D. Campisi**²⁰, A. G. G. M. Tielens, W. Dononelli, *The Effect of PAH Adsorption on MgO Schottky Vacancies on Forsterite 2024*, in preparation.

Conferences, Workshops, Schools, Others

Invited Talks

23–20/02/2024 NanoSpace Edinburgh Meeting²⁶ 2024, Edinburgh, UK. Invited by the SOC.

11–14/09/2023 Congresso Nazionale di Astrochimica Protoplanetaria (Astrochemistry Workshop)²⁴, Trieste, Italy, Invited by the SOC.

12–16/06/2023 Workshop on Interstellar Catalysis²⁵, Fuglsøcentret, Aarhus, Denmark, Invited by Prof. Dr. Liv. Hornekær.

10–14/06/2023 Center for Astrochemical Studies (CAS) Seminar²⁵, Max Planck Institute for Extraterrestrial Physics (MPE), Garching, Germany, Invited by Prof. Dr. Paola Caselli.

Featured Talks

28/08/2023 36th European Conference on Surface Science²⁶ (ECOSS36), Łódź, Poland.

Seminars

25/06/2020 UCF AVS Astrochemistry Webinar series²⁵, University of Central Florida Chapter.

27/11/2019 *Astrochemistry and the Molecular Universe Seminar*²⁵, Liceo Scientifico Albert Einstein, Palermo, Italy.

22/05/2019 *The Molecular Universe Seminar*²⁵, Milan University, Milan, Italy.

Contributed Talks

5–9/06/2023 Chemical Processes in Solar-type Star-Forming Regions conference²⁶, Toulouse, France.

5–9/09/2022 CosmicPAH 2022 conference²⁵, Aarhus, Denmark.

21–25/08/2022 ACS fall 2022 conference²⁷, Chicago, US.

08/03/2021 The EUROPAH conference (online conference)²⁵, Aarhus University, Aarhus, Denmark.

02/02/2021 Dutch Astrochemistry Network Meeting: The Aromatic Universe²⁵, Radboud University, Nijmegen, the Netherlands.

²⁴ Presenting a review of Computational Astrochemistry.

²⁵ Presenting the work of my PhD thesis (10).

²⁶ Presenting project in preparation (12).

²⁷ A talk on material science.

24-23/09/2019 PAHRTEA - PAH Research: Theory, Experiments in an Astronomical context²⁸; EUROPAH conference, Radboud University, Nijmegen, the Netherlands.

14-15/03/2019 The NAC (Nederlands Aardwetenschappelijk Congres) conference²⁷, Utrecht, the Netherlands.

02/11/2018 Dutch Astrochemistry Network Meeting: The Aromatic Universe²⁹, Radboud University, Nijmegen, the Netherlands.

26-28/09/2018 EUROPAH mid-term review³⁰, Heriot-Watt University, Edinburgh, United Kingdom.

26-31/08/2018 34th European Conference on Surface Science²⁹ (ECOSS34), Aarhus, Denmark.

Posters

27-28/01/2021 Origins 2021 Online Conference²⁵, Utrecht University, Utrecht, the Netherlands.

14-15/11/2019 Holland Research School of Molecular Chemistry, Lustrum Symposium^{28,31}, Royal Tropical Institute, Amsterdam, the Netherlands.

24-28/06/2019 EUROPAH Summer School "PAHs in extreme environments"²⁸, Paul Sabatier University, Toulouse, France.

03/2019 Energetic Processing of Large Molecules (EPoLM-4) Conference²⁸, CSIC headquarters, Madrid, Spain.

11-15/06/2018 CPHDUST2018 conference^{29,30}, Copenhagen, Denmark.

02/05/2018 PEPSci meeting²⁵, Leiden University, Leiden, the Netherlands.

11-16/03/2018 Winter School: Volatile elements in the Solar System²⁵, The Ecole de Physique des Houches, Les Houches, France.

15/03/2018 The Netherlands Aardwetenschappelijk Congres (NAC)^{25,30}, NH Koningshof, Veldhoven, the Netherlands.

6-20/09/2017 EUROPAH Introductory Training Event²⁵: Introductory Training, Public Engagement, Scanning Probe Microscopy, Aarhus University, Aarhus, Denmark.

Others

9-11/11/2022 Hybrid Network Meeting of the Alexander von Humboldt Foundation 2022, Goethe University, Frankfurt, Germany.

5-7/10/2021 International Symposium on Correlated Electrons (SymCorrel21), online symposium organized by Munich Center for Quantum Science and Technology, München, Germany.

7-11/09/2020 EUROPAH Leadout Training, Webinar organized by Aarhus University and University of Münster, Aarhus and Münster, Denmark and Germany.

25/09/2019 EUROPAH workshop "Public Engagement", Radboud University, Nijmegen, the Netherlands.

30/09/2018-01/10/2018 EUROPAH workshop "Innovation and Entrepreneurship", University of Liverpool, Liverpool, U.K.

25/09/2018 EUROPAH workshop "PAHs, Nanoparticles and the Terrestrial Environment", Heriot-Watt University, Edinburgh, U.K.

2-9/04/2018 EUROPAH Summer School "PAHs in the Interstellar Medium", The Ecole de Physique des Houches, Les Houches, France.

4-6/12/2017 Workshop on Material Science Codes on innovative HCP architectures: targeting exscale, CINECA, Casalecchio di Reno (Bo), Italy.

2/12/2017-30/11/2017 PhD introductory event "Time management and Effective communication", Leiden University, Leiden and Noordwijk, the Netherlands.

References

- 1) **Prof. Dr. Johannes Kästner**, Institute for Theoretical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany, phone: +49 711 68564473. Email: kaestner@theochem.uni-stuttgart.de
- 2) **Prof. Dr. Alexander G. G. M. Tielens**, Leiden Observatory, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, the Netherlands, phone: +31 71 527 8465. Email: tielens@strw.leidenuniv.nl
- 3) **Prof. Dr. Inge Loes ten Kate**, Institute of Astronomy, University of Amsterdam and Utrecht University, Science Park 904 and Princetonlaan 8a, 1090 GE Amsterdam and 3584 CB Utrecht, the Netherlands. Email: i.l.tenkate@uva.nl / i.l.tenkate@uu.nl

²⁸ Presenting the work of publication (5).

²⁹ Presenting the work of publication (7).

³⁰ Presenting the work of publication (8).

³¹ Poster presented by a collaborator. I did not attend the conference