Dr. Dario Campisi
Institute for Theoretical Chemistry, University of Stuttgart, Pfaffenwaldring 55,
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Education

(14/09/2021) - PhD in Astronomy
Leiden Observatory/Astronomy Department, Leiden University, Leiden, the Netherlands.
Funded by Marie Curie H2020 ITN EuroPAH and Dutch Astrochemistry Network.
Thesis: "*Interstellar Catalysts and the PAH Universe*".
Supervisor: Prof. Dr. Alexander G. G. M. Tielens.
Co-supervisors: Prof. Dr. Inge Loes ten Kate and Dr. Thanja Lamberts.

(10/03/2017) - MSc in Chemistry
Department of Physics and Chemistry, University of Palermo, Palermo, Italy.
Thesis: "*Computational Study of the Catalytic Effects of Frustrated Lewis Pair-Based Materials*".
Supervisor: Prof. Dr. Dario Duca.
Co-supervisor: Dr. Remedios Cortese.

(20/10/2014) - BSc in Chemistry
Department of Physics and Chemistry, University of Palermo, Palermo, Italy.
Thesis: "*Optimization of Suzuki Reaction for the Synthesis of Derivatives of Interest in Optoelectronic*".
Supervisor: Prof. Dr. Michelangelo Gruttadauria.
Co-supervisor: Prof. Dr. Francesco Giacalone.

Employment and Work Experience

(30/09/2024 - 1/10/2022) - Head of Astrochemistry[#], Postdoc, Humboldt fellow
Institute for Theoretical Chemistry, University of Stuttgart, Stuttgart, Germany.
Supervisor: Prof. Dr. Johannes Kästner.
([#]) Fixed-term contract.

(31/08/2022 - 1/10/2021) - Postdoctoral Researcher
Chemistry Department, The University of Chicago, Chicago, USA.
Supervisor: Prof. Dr. Laura Gagliardi.

(27/09/2021 - 28/08/2017) - Early Stage Researcher (H2020 MSCA ITN EuroPAH)
Leiden Observatory, Leiden University, Leiden, the Netherlands.
Supervisor: Prof. Dr. Alexander G. G. M. Tielens.

- (3 Months) Secondment at Milan University, Milan, Italy. Project: "Periodic DFT approaches: SIESTA code". Supervisor: Prof. Dr. Rocco Martinazzo.
- (1 Month) Secondment at Graphic Science, Bristol, UK. Project: "Outreach Exhibition". Supervisor: Mr. Ben Johnson.
- (2 Months) Secondment at Aarhus University, Aarhus, Denmark. Project: "Machine Learning Approaches". Supervisor: Prof. Dr. Bjørk Hammer.

(11/07/2017 - 11/03/2017) - Voluntary Researcher
Department of Physics and Chemistry, University of Palermo, Palermo, Italy.
Supervisor: Prof. Dr. Dario Duca.

(01/02/2013 - 01/11/2012) - Undergraduate Internship
Institute for the Study of Nanostructured Materials, National Research Council (CNR), Palermo
Supervisor: Dr. Maria Luisa Testa.

Grants, Fellowships, Awards

(2024) Seal of Excellence for the submitted European Marie Curie Postdoctoral Fellowship proposal, 101150786-FIPAH, University of Stuttgart, Germany.

(30/09/2024 - 1/10/2022) Humboldt Research Fellowship for postdocs (€86,280), University of Stuttgart, Stuttgart, Germany.

(2022) Seal of Excellence for the submitted Global Marie Curie Postdoctoral Fellowship proposal, 101064156- DFT-DMET-ML, Aarhus University, Denmark.

(22/08/2022 - 01/01/2018) Computational Time (~1,400,000 core hours) on HPC SurfSara (the Netherlands) and CINECA (Italy). Granted Projects: EINF-154, EINF-1888, UARP, AFPF, IPCM, IPCM2, PFCM and APF.

(27/08/2020 - 28/08/2017) Marie Curie Fellowship for PhD students (H2020 MSCA-ITN EuroPAH, ~€103,680, grant number: 722346, PI: Prof. Dr. A.G.G.M. Tielens), Leiden University, Leiden, the Netherlands.

Teaching/supervising experience

(2024 - 2022) - Head of Astrochemistry[#], University of Stuttgart, Germany

- Management and supervision of astrochemistry/computational chemistry projects in Prof. Dr. Johannes Kastner's group.
- Delivered tutorial sessions on computational chemistry codes tailored for solid-state chemistry to PhD students, and postdocs in Prof. Dr. Johannes Kastner's group.
- Supervised a BSc student and two paid undergraduate projects (A. Riffelt and S. Haid), currently mentoring an MSc student (T. Hähnel).

Note: Successfully supervised the BSc thesis of student A. Riffelt, resulting in her graduation. Her dissertation was awarded the 500 euros IC SimTech award for outstanding thesis.

(#) Fixed-term contract.

(2022 - 2021) - Teaching Assistant, the University of Chicago, USA

- Delivered a ten-lecture series, totaling 10 hours, on quantum chemistry to undergraduate (all years), PhD students, and postdocs associated with the Chicago Centre for Theoretical Chemistry.
- Supervised the BSc internship project of M. Pinheiro.
- Supervised the collaborative postdoc project of Dr. A. Sarkar.
- Supervised M. N. McCabe's PhD project at Leiden University.

(2021 - 2020) - Teaching Assistant, Leiden University, the Netherlands

- Teaching Assistant for the Astronomical Spectroscopy MSc course for two years, conducting 4-hour simulation classes each year. Reviewed reports and graded assignments for a class of approximately 20 students annually.

- Teaching Assistant for the Modern Astronomical and Physics Research courses in the Astronomy program's final year of the BSc online program. Responsibilities included managing class activities, developing schedules and course materials, moderating group discussions, reviewing reports and posters, and grading assignments for approximately 60 students. The course, totaling 28 hours, was taught for only one year.

(27/11/2019) - Lecturer, High School, Palermo, Italy

- Delivered three Astrochemistry classes, totaling 3 hours, to Year 11 high school students, about 80 students, at Albert Einstein Scientific Lyceum in Palermo. Conducted three sessions on astrochemistry, including class lectures and group discussions.

Public Engagement

(27/04/2023) - Girls' Day, University of Stuttgart, Stuttgart, Germany.

- Organized the astrochemistry section of an open day for high school girls to attract them to science.

(27-18/07/2019) - EUROPAH Astrochemistry Pop-up shop, The Galleries, Bristol, UK.

- Organized a science exhibition open to all ages, featuring a pop-up shop in collaboration with EuroPAH fellows.

(19/11/2019) - Astronomy on TAP, EuroPAH: "A network of early-stage researchers", Grand Cafe De Burcht, Leiden, the Netherlands.

- Delivered a public presentation on the initiatives and accomplishments of the EuroPAH network.

(29/09/2018) - Explorathon, Heriot-Watt University, Edinburgh, U.K..

- Organized a poster and video exhibition section highlighting the scientific activities of EuroPAH to the public.

(27/08/2020 - 30/09/2017) - Management of EuroPAH Public Blog, http://www.europah.eu/.

- Wrote public blogs about the activities of the EuroPAH network.

Organization of Scientific Meetings

(1/09/2023 - 28/08/2023) - Organizer and Chair of a Mini-Symposium "Surface Astrochemistry" at the 36th European Conference on Surface Science (ECOSS36), Lodz, Poland.

- Responsible for coordinating schedules, evaluating abstracts, assigning talks/posters, and chairing the session.

(24-23/09/2019) - Member of Scientific Organizing Committee (SOC) PAHRTEA - PAH Research: Theory, Experiments in an Astronomical Context; EUROPAH conference, Radboud University, Nijmegen, The Netherlands.

- Responsible for coordinating schedules, evaluating abstracts, and assigning talks/posters.

Memberships

- **Member of COST (European Cooperation in Science and Technology) (since 2024):** COST is a renowned funding Organization dedicated to supporting research and innovation networks across Europe.

- **Member of the Alexander von Humboldt Network (since 2022):** The Alexander von Humboldt Network is a prestigious organization fostering international academic and research collaborations.

Referee Duties

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

Publications

During my master's, PhD studies, and postdoctoral research positions, I have authored and co-authored publications in computational chemistry applied to astrochemistry, planetary science, and materials chemistry.

Peer-reviewed journal articles

1) **D. Campisi***, T. Lamberts, N. Y. Dzade, R. Martinazzo, I. L. ten Kate, A. G. G. M. Tielens, *Adsorption of Polycyclic Aromatic Hydrocarbons and C_{60} 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. Campisi[b]**, N. Zhao, B. Cheng, G. L. Grocke, T. Ma, A. S. Filatov, L. Gagliardi, J. S. Anderson*, *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. Campisi[c]**, 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. LaVerne*, *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. Campisi[a]**, J. C. Broxterman, E. Reusch, A. Bodi and J. Bouwman*, *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. Campisi***, 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, 2770-27812021. https://doi.org/10.1021/acs.jpca.1c02326

6) **D. Campisi*** and A. Candian*, *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

7) **D. Campisi***, 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

8) R. Cortese, **D. Campisi[c]**, A. Prestianni and D. Duca*, *Alkane Dehydrogenation on Defective BN Quasi-Molecular Nanoflakes: DFT Studies*, Molecular Catalysis 2020, 493, 110891. https://doi.org/10.1016/j.mcat.2020.110891

9) R. Cortese, **D. Campisi**[c] and D. Duca*, *Hydrogen Arrangements on Defective Quasi-Molecular BN Fragments*, ACS omega, 2019, 4, 14849-14859. https://doi.org/10.1021/acsomega.9b01445

PhD thesis:

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

Submitted:

11) **D. Campisi***, A. G. G. M. Tielens, W. Dononelli, *The Role of Point Defect Reconstructions and Polycyclic Aromatic Hydrocarbons (PAHs) in Silicate Dust Preservation* 2024, submitted in MNRAS.

12) **D. Campisi***, F. Tonolo, S. Alessandrini, J. Perrero, N. Balucani, *Computational Astrochemistry - Journey Towards the Molecular Universe* 2024, Conference Proceeding chapter, submitted in Mem. S.A.It.

In preparation:

13) **D. Campisi***, P. Caselli, and J. Kästner, *Tunneling Toward Interstellar PAHs: O and H's Quantum Leap* 2024, in preparation; submission in Nature Astronomy pending.

14) F. Kruczkiewicz, B.M. Giuliano, **D. Campisi**[c], A. A. Gavdush, K. I. Zaytsev, G. A. Komandin, A. Ivlev, F. Ribeiro, P. Caselli*, *Far-Infrared Spectroscopy of Cryogenic N_2 and O^2 Molecular Solids at Low Pressure* 2024, submission in Astronomy & Astrophysics pending.

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

16) A. Riffelt, J Kästner, **D. Campisi***, *Formation of Formamide on Forsterite* 2024, in preparation.

(*) Corresponding author/project leader.
([a]) Contribution as PhD project supervisor (M. N. McCabe).
([b]) Contribution as postdoctoral project supervisor (A. Sarkar).
([c]) Responsible for and performer of DFT Simulations and drafting of the theoretical part of the paper.

Research skills

- **Quantum Chemistry Codes:** ORCA and Gaussian (Gas-Phase). Siesta, VASP, GPAW (Solid State).
- **Machine Learning Potentials**: GOFEE (Global Optimisation with first principle energy expressions) and Catlearn (ML potential for Transition States Search).
- **Reactivity:** Kinetic rates and Quantum tunneling (Instanton, Eckart, and Bell).
- **Theories:** Density Functional Theory, Coupled Cluster, Møller–Plesset perturbation theory, Ab Initio Molecular Dynamics.
- **Simulation Environments:** Python Atomistic Simulation Environment (ASE) and CHEMSHELL DL-FIND.
- **Others:** METADISE (Interface and Surface preparation).
- **Programming:** Python and bash.

Languages

Italian: Native Language.

English: Fluent (Evaluated at the Language Centre at Leiden University and the University of Chicago).

Conferences and presentations

Invited Talks

(23-20/02/2024) - NanoSpace Edinburgh Meeting 2024, Edinburgh, UK. Title: Tunneling Toward Interstellar PAHs: O and H's Quantum Leap**.**

(14-11/09/2023) - Congresso Nazionale di Astrochimica Protoplanetaria (Astrochemistry Workshop), Trieste, Italy. Title: Super-Oxygenation of Naphthalene: The Break-Down Reaction.

(16-12/06/2023) - Workshop on Interstellar Catalysis, Fuglsøcentret, Aarhus, Denmark. Title: Interaction of PAHs on olivinic grains: A quantum chemistry perspective.

(14-10/06/2023) - Centre for Astrochemical Studies (CAS) Seminar, Max Planck Institute for Extraterrestrial Physics (MPE), Garching, Germany. Title: Interstellar Catalysts and the PAH Universe.

Featured Talks

(28/08/2023) - 36th European Conference on Surface Science (ECOSS36), Łodz, Poland. Title: Super-Oxygenation of Naphthalene: The Break-Down Reaction.

Seminars

(25/06/2020) - UCF AVS Astrochemistry Webinar series, University of Central Florida, Orlando, USA. Title: Delivery of PAHs in the Early Solar System: Forsterite as Space Shuttle.

(27/11/2019) - Astrochemistry Seminar, Albert Einstein Scientific Lyceum, Palermo, Italy. Title: The Molecular Universe.

(22/05/2019) - Astrochemistry Seminar, Milan University, Milan, Italy. Title: The Molecular Universe.

Contributed Talks

(9-5/06/2023) Chemical Processes in Solar-type Star-Forming Regions conference, Toulouse, France. Title: Super-Oxygenation of Naphthalene: The Break-Down Reaction.

(9-5/09/2022) CosmicPAH 2022 conference, Aarhus, Denmark. Title: The Effect of PAH Adsorption on MgO Schottky Vacancy in Forsterite: A Machine-Learned Surrogate Model.

(25-21/08/2022) ACS fall 2022 conference, Chicago, USA. Title: Role of metal selection in the radiation stability of isostructural M-UiO-66 metal-organic frameworks.

(**08/03/2021) The EUROPAH conference (online conference)**, Aarhus University, Aarhus, Denmark. Title: The Interaction of PAHs and C_{60} with Forsterite: Machine Learning and DFT-D4 studies.

(02/02/2021) Dutch Astrochemistry Network Meeting: The Aromatic Universe, Radboud University, Nijmegen, the Netherlands. Title: The Interaction of PAHs and C_{60} with Forsterite.

(24-23/09/2019) PAHRTEA - PAH Research: Theory, Experiments in an Astronomical context; **EUROPAH conference**, Radboud University, Nijmegen, the Netherlands. Title: Prebiotic Activity of Forsterite: PAHs Hypothesis.

(15-14/03/2019) The NAC (Nederlands Aardwetenschappelijk Congres) conference, Utrecht, the Netherlands. Title: Aqueous Alteration of Forsterite: The Face Matters.

(02/11/2018) Dutch Astrochemistry Network Meeting: The Aromatic Universe, Radboud University, Nijmegen, the Netherlands. Title: Effect of Stone Wales defect in the formation of interstellar H_2.

(31-26/08/2018) 34th European Conference on Surface Science (ECOSS34), Aarhus, Denmark. Title: Superhydrogenation of pentacene: the role of zigzag-edges in H_2 formation.

Posters

(28-27/01/2021) - Origins 2021 Online Conference, Utrecht University, Utrecht, the Netherlands. Title: DFT-D4 Investigation of Fullerene and PAHs on (010) Forsterite Surfaces.

(15-14/11/2019) - **Holland Research School of Molecular Chemistry**, Lustrum Symposium, Royal Tropical Institute, Amsterdam, the Netherlands. Title: "Frustrated Carbon Pairs": From Stone Wales formation to astrocatalysis of H_2.

(28-24/06/2019) - EUROPAH Summer School "PAHs in extreme environments", Paul Sabatier University, Toulouse, France. Title: Frustrated Carbon Pairs": From Stone Wales formation to astrocatalysis of H_2.

(03/2019) - Energetic Processing of Large Molecules (EPoLM-4) Conference, CSIC headquarters, Madrid, Spain. Title: Frustrated Carbon Pairs": From Stone Wales formation to astrocatalysis of H_2.

(15-11/06/2018) - CPHDUST2018 conference, Copenhagen, Denmark. Title: Investigation of the hydrogenation of pentacene.

(02/05/2018) - PEPSci meeting, Leiden University, Leiden, the Netherlands. Title: DFT investigations of PAHs in meteorites.

(16-11/03/2018) - Winter School: Volatile Elements in the Solar System, The Ecole de Physique des Houches, Les Houches, France. Title: DFT investigations of PAHs in meteorites.

(**15/03/2018) - The Nederlands Aardwetenschappelijk Congres (NAC)**, NH Koningshof, Veldhoven, the Netherlands. Title: DFT investigations of PAHs in meteorites.

Other Meetings

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

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

(11-7/09/2020) - 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"**, the 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.

(6-4/12/2017) - 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

- **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

- **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

- **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, phone:+31 30 253 5065. Email: i.l.tenkate@uu.nl