

## CV

### Personal information

**Name:** Dr. Dario Campisi

**Affiliation:** University of Stuttgart, Institute for Theoretical Chemistry, Pfaffenwaldring 55, 70569 Stuttgart, Germany

**Nationality:** Italian

**Email:** [campisi@theochem.uni-stuttgart.de](mailto:campisi@theochem.uni-stuttgart.de)

**ORCID:** 0000-0001-8981-8738

**Languages:** Italian (Mother Tongue) and English (Fluent)<sup>1</sup>

### Education and Training:

**14/09/2021 Ph.D.** in Astronomy<sup>2</sup> (within MSCA-ITN EuroPAH), Leiden Observatory/Astronomy Department, 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, Physics and Chemistry Department, 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, Physics and Chemistry Department, 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 Astrochemistry<sup>3</sup>, 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.

**27/09/2021-28/08/2017** Early Stage Researcher<sup>4</sup>, 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 Month) 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** Undergraduate Internship, National Research Council (CNR) - Institute for the Study of Nanostructured Materials 153, Via Ugo La Malfa, 90146 Palermo, Italy, [www.ismn.cnr.it](http://www.ismn.cnr.it).

### Fundings and Awards

**03/2024** Seal of Excellence for the Submitted European Marie Curie Postdoctoral Fellowship proposal, 101150786-FIPAH, Stuttgart University, Germany.

**30/09/2024-1/10/2022** Humboldt Research Fellowship<sup>5</sup> for Postdocs, University of Stuttgart, Stuttgart, Germany.

**21/03/2022** Seal of Excellence for the Submitted Global Marie Curie Postdoctoral Fellowship proposal, 101064156- DFT-DMET-ML, Aarhus University, Denmark.

<sup>1</sup> Certified at the University of Chicago Language Center.

<sup>2</sup> The doctoral program in the Netherlands is 4 years.

<sup>3</sup> Fixed-term position. This is an internal project management position in the Kästner group.

<sup>4</sup> Position that implies research, training, secondments, outreach, teaching assistant.

<sup>5</sup> Prestigious fellowship in Germany

**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 Day<sup>6</sup>, University of Stuttgart, Stuttgart, Germany

**18-27/07/2019** EUROPAH Astrochemistry pop-up shop<sup>7</sup>, The Galleries, Bristol, UK.

**19/11/2019** Astronomy on TAP, euroPAH<sup>8</sup>: "*A network of early-stage researchers*", Grand Cafe De Burcht, Burgsteeg 14, 2312 JS Leiden, the Netherlands.

**29/09/2018** Explorathon<sup>9</sup>, Heriot-Watt University, Edinburgh, U.K..

**27/08/2020-30/09/2017** Management of EuroPAH Public Blog<sup>10</sup>, <http://www.europah.eu/>.

### (Co-)organization of Scientific Meetings

**1/09/2023-28/08/2023** Organizer<sup>11</sup> and Chair of the Mini-Symposium "*Surface Astrochemistry*" at the 36th, European Conference on Surface Science (ECOSS36), Lodz, Poland.

**23-24/09/2019** SOC<sup>12</sup> 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 HIWI<sup>13</sup> student projects, Institute for Theoretical Chemistry, University of Stuttgart, Stuttgart, Germany. *Student: Annalena Riffelt and Severin Haid.*

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<sup>6</sup> Management of the astrochemistry section.

<sup>7</sup> 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.

<sup>8</sup> Talk in a public space about the activities of EuroPAH network.

<sup>9</sup> 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.

<sup>10</sup> I wrote several blogs related to the EuroPAH activities and my research projects.

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

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

<sup>13</sup> A paid research internship student.

**31/05/2023-01/11/2022** Supervision of BSc Thesis Student Project<sup>14</sup>, Institute for Theoretical Chemistry, University of Stuttgart, Stuttgart, Germany. *Student: Annalena Riffelt.*<sup>15</sup>

**01/08/2022-01/10/2021** Supervision of Postdoc Project<sup>16</sup>, Chemistry Department, the University of Chicago, Chicago, US. *Postdoc: Arup Sarkar.*

**01/08/2022-01/02/2022** Supervision of Undergraduate Student Project<sup>17</sup>, Chemistry Department, the University of Chicago, Chicago, US. *Student: Manuela Pinheiro.*

**12/11/2021-01/09/2020** Supervision of Graduate Student Project<sup>18</sup>, Leiden Observatory, Leiden University, Leiden, the Netherlands. *Student: Morgan McCabe.*

## **Publications**

During my master's, PhD studies, and two years of postdoctoral research, I have authored and co-authored publications in the fields of Astrochemistry/Cosmochemistry, Materials Science, and Catalysis, along with completing a PhD thesis. The aforementioned publications are detailed and discussed as follows:

## **Peer-reviewed journal articles**

### ***Astrochemistry and Cosmochemistry:***

**1) D. Campisi<sup>19</sup>**, 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) M. N. McCabe**, P. Hemberger, **D. Campisi<sup>20</sup>**, J. C. Broxterman, E. Reusch, A. Bodi and J. Bouwman<sup>18</sup>, *Formation of phenylacetylene and benzocyclobutadiene in the ortho-benzynes + acetylene reaction*, Physical Chemistry Chemical Physics **2022**, 24, 1869–1876. <https://doi.org/10.1039/D1CP05183K>

**3) D. Campisi<sup>19</sup>**, 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>

**4) D. Campisi<sup>19</sup>** and A. Candian<sup>19</sup>, *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>

**5) D. Campisi<sup>19</sup>**, 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>

### ***Material Science:***

**6) L. Wang**, R. J. Papoular, N. E. Horwitz, J. Xie, A. Sarkar, **D. Campisi<sup>21</sup>**, N. Zhao, B. Cheng, G. L. Grocke, T. Ma, A. S. Filatov, L. Gagliardi, J. S. Anderson<sup>19</sup>, *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>

**7) A. M. Hastings**, M. Fairley, M. C. Wasson, **D. Campisi<sup>22</sup>**, 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<sup>19</sup>, *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>

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

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

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

<sup>17</sup> Supervision of an Internship project.

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

<sup>19</sup> Corresponding author/Project leader.

<sup>20</sup> I supervised M.N. McCabe's calculations and revised the theoretical part of the manuscript.

<sup>21</sup> I supervised postdoc A. Sarkar's calculations and wrote the theoretical part of the article.

<sup>22</sup> I performed calculations and wrote the theoretical part of the article.

### Catalysis:

8) R. Cortese, **D. Campisi**<sup>23</sup>, A. Prestianni and D. Duca<sup>19</sup>, *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**<sup>23</sup> and D. Duca<sup>19</sup>, *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**<sup>19</sup>, *Interstellar Catalysts and the PAH universe*, PhD thesis, **2021**, ISBN: 9789464192957. <https://hdl.handle.net/1887/3210124>

*Note: In 2023, I worked on and submitted proposals for four grant application schemes: VENI (NWO), Marie Curie Postdoctoral Fellowship 2023, ERC Starting Grant 2024, and The Branco Weiss Fellowship Society in Science. The Branco Weiss Fellowship can be incorporated into any tenure track positions if funded.*

### In preparation

11) **D. Campisi**<sup>19</sup>, A. G. G. M. Tielens, W. Dononelli, *The Effect of PAH Adsorption on MgO Schottky Vacancies on Forsterite* **2024**, Completed draft; submission in *MNRAS* pending

12) **D. Campisi**<sup>19</sup>, P. Caselli, and J. Kästner, *Tunneling Toward Interstellar PAHs: O and H's Quantum Leap* **2024**, Completed draft; submission in *Nature Astronomy* pending

13) **D. Campisi**<sup>19</sup>, *Formation of Formamide on Forsterite* **2024**, in preparation

14) S. Haid, K. Gugeler, J. Kästner, **D. Campisi**<sup>19</sup>, *Super-Hydrogenation of Indene* **2024**, in preparation

15) F. Kruczkiewicz, B.M. Giuliano, **D. Campisi**<sup>22</sup>, A. A. Gavdush, K. I. Zaytsev, G. A. Komandin, A. Ivlev, F. Ribeiro, P. Caselli<sup>19</sup>, *Far-Infrared Spectroscopy of Cryogenic N<sub>2</sub> and O<sub>2</sub> Molecular Solids at Low Pressure* **2024**, in preparation

### Conferences, Workshops, Schools, Others

#### Invited Talks

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

**11-14/09/2023** Congresso Nazionale di Astrochimica Protoplanetaria (Astrochemistry Workshop)<sup>24</sup>, Trieste, Italy. Title: *Super-Oxygenation of Naphthalene: The Break-Down Reaction*.

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

**10-14/06/2023** Center 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<sup>25</sup> (ECOSS36), Łódź, Poland. Title: *Super-Oxygenation of Naphthalene: The Break-Down Reaction*.

#### Seminars

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

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

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

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<sup>23</sup> I performed the theoretical calculations and revised the final draft of the manuscript.

<sup>24</sup> Presenting a review of Computational Astrochemistry.

<sup>25</sup> Presenting project in preparation (12).

## Contributed Talks

- 5-9/06/2023** Chemical Processes in Solar-type Star-Forming Regions conference, Toulouse, France.  
**5-9/09/2022** CosmicPAH 2022 conference, Aarhus, Denmark.  
**21-25/08/2022** ACS fall 2022 conference, Chicago, US.  
**08/03/2021** The EUROPAH conference (online conference), Aarhus University, Aarhus, Denmark.  
**02/02/2021** Dutch Astrochemistry Network Meeting: The Aromatic Universe<sup>25</sup>, Radboud University, Nijmegen, the Netherlands.  
**24-23/09/2019** PAHRTEA - PAH Research: Theory, Experiments in an Astronomical context; EUROPAH conference, Radboud University, Nijmegen, the Netherlands.  
**14-15/03/2019** The NAC (Nederlands Aardwetenschappelijk Congres) conference, Utrecht, the Netherlands.  
**02/11/2018** Dutch Astrochemistry Network Meeting: The Aromatic Universe, Radboud University, Nijmegen, the Netherlands.  
**26-31/08/2018** 34th European Conference on Surface Science (ECOSS34), Aarhus, Denmark.

## Posters

- 27-28/01/2021** Origins 2021 Online Conference, Utrecht University, Utrecht, the Netherlands.  
**14-15/11/2019** Holland Research School of Molecular Chemistry, Lustrum Symposium, Royal Tropical Institute, Amsterdam, the Netherlands.  
**24-28/06/2019** EUROPAH Summer School "PAHs in extreme environments", Paul Sabatier University, Toulouse, France.  
**03/2019** Energetic Processing of Large Molecules (EPoLM-4) Conference, CSIC headquarters, Madrid, Spain.  
**11-15/06/2018** CPHDUST2018 conference, Copenhagen, Denmark.  
**02/05/2018** PEPSci meeting, Leiden University, Leiden, the Netherlands.  
**11-16/03/2018** Winter School: Volatile Elements in the Solar System, The Ecole de Physique des Houches, Les Houches, France.  
**15/03/2018** The Netherlands Aardwetenschappelijk Congres (NAC), NH Koningshof, Veldhoven, the Netherlands.  
**6-20/09/2017** EUROPAH Introductory Training Event: 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](mailto: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](mailto: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@uu.nl](mailto:i.l.tenkate@uu.nl)