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## Interstellar catalysts and the PAH universe

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## LIST OF PUBLICATIONS

### First Author

1. **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, 2770-2781. DOI: <https://doi.org/10.1021/acs.jpca.1c02326>
2. **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. DOI: <https://doi.org/10.1039/C9CP06523G>
3. **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. DOI: <https://doi.org/10.1039/C9CP05440E>

### Contributed Author

1. R. Cortese, **D. Campisi**, A. Prestianni and D. Duca\*, *Alkane Dehydrogenation on Defective BN Quasi-Molecular Nanoflakes: DFT Studies*, **Molecular Catalysis** **2020**, 493, 110891. DOI: <https://doi.org/10.1016/j.mcat.2020.110891>

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

## **In Preparation/Submitted**

1. **D. Campisi**\*, N. Y. Dzade, R. Martinazzo, I. L. ten Kate, T. Lamberts and A. G. G. M. Tielens, *Adsorption of PAHs and C<sub>60</sub> onto Forsterite: C-H Bond Activation by the Schottky Vacancy*
2. **D. Campisi**\*, W. Dononelli, B. Hammer and A. G. G. M. Tielens, *Finding the stable location of a MgO vacancy in Forsterite (Mg<sub>2</sub>SiO<sub>4</sub>) using global optimization with first principles energy expressions*

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## CURRICULUM VITAE

I was born on one of the hottest Saturdays of summer in Italy, specifically, on the 14th of June 1986 in Palermo (Sicily). My mom was a chemical expert in a clinical analysis lab and she infused me her love for organic chemistry. On top of this, I have been always fascinated by computers and programming. My first computer was a commodore 64 in which I learned the basics of BASIC code. Later on, in middle school, my teacher, Graziella Solina, introduced me to science and math. So I decided to be enrolled in scientific high school (Liceo Scientifico) in which my teacher Elvira Piccione mentored me and inspired me to love chemistry and astronomy.

After high school, I felt lost and I was dealing with some personal and family issues that led me to be enrolled initially in a geology bachelor course which I left after one year and a half since I did not feel that was a path to follow. Later on, when I was about 24, I decided to be enrolled in a chemistry bachelor course (Laurea Triennale) at Palermo University. The chemistry bachelor course in Italy was too focused on the experimental aspect of chemistry. On top of this, the faculty members discouraged students from undertaking internships based on research but rather they pushed them to consider analytical chemistry careers in the industry. This made me realized that I did not want to be a lab mouse but rather I was curious about researching and discovering. Hence, I did an internship in the national research council (CNR) and I carried out an experimental thesis in organic chemistry.

I have not been happy with my bachelor's course and I was reluctant to proceed with a master's course in chemistry since I needed a more open-minded environment that allows exploring different disciplines. However, I knew that I wanted to have a PhD, and being enrolled in the chemistry master course (Laurea Magistrale) at Palermo University was a smart choice. Here, I have been introduced to theoretical chemistry, spectroscopy, and catalysis — three disciplines that I completely fell in love with. So, I deci-

ded to carry out a thesis in computational chemistry applied to catalysis in Dario Duca's group, co-supervised by Remedios Cortese. Furthermore, they introduced me to astrochemistry and the idea of catalysis in space. I got my master with the top grade and I started to search for PhD positions.

When I found advertised several positions in astrochemistry within a Marie Curie network called EUROPAH, I decided to apply without second thoughts. So, I have been introduced to my co-supervisor, Inge Loes ten Kate, and my promotor, Xander Tielens, and they decided to accept me as PhD candidate at Leiden University as well as one of the Early Stage Researcher (ESR) of the Marie Curie ITN-EUROPAH network.

During the first EUROPAH training event at Aarhus University, which I attended in the second week of my PhD, I have been asked to run small calculations in support of the final poster. Here, I gave a good impression to Liv Hornekær (Aarhus University) who asked me to collaborate with her and with Rocco Martinazzo (Milan Universe). This collaboration gave birth to the results of chapter 2 of this thesis. In my first two years, I have been in contact with Alessandra Candian (my office mate) who mentored me and collaborated with me in chapter 3 of this thesis.

The first part of my PhD thesis has been focused on the interstellar medium and gas-phase processes. However, I wanted to explore also solar system and this resulted in my final two chapters with the collaboration of Rocco Martinazzo, Thanja Lamberts who has become officially my co-supervisor, Nelson Dzade at Cardiff University, and Inge Loes ten Kate. Furthermore, during the time spent in the EUROPAH network, I had the privilege to get broad training thanks to several organized workshops, conferences, and outreach activities. I also have been seconded to Milan University for four months in which I received training on periodic calculations. I spent a month in Bristol, UK, to develop an outreach project that gave birth to a pop-up shop. I have been part of the Social Organizing Committee (SOC) of the "PAH Research: Theory, Experiments in an Astronomical context" conference organized by EUROPAH's ESRs. Finally, I have been seconded to Aarhus University in Bjørk Hammer's group in which I received training on machine learning. Unfortunately, my secondment has been interrupted by the COVID-19 pandemic which led me to continue remotely. Finally, I will be appointed, this fall (2021), as a post-doc in Laura Gagliardi's theoretical chemistry group at Chicago University. I will work on applying and developing quantum chemical methods based on wave function methods that will be tested on the forsterite models studied in this thesis as well as on actinide chemistry.

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In four years of my PhD, I have met many brilliant and inspiring people. I am afraid that I might forget to acknowledge some of them. Hence, if your name is not in this acknowledgment, I thank you because somehow you provided an indirect contribution to finalize this thesis. Every person I met during my PhD helped me to grow as a scientist.

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