Interstellar catalysts and the PAH universe

Campisi, D.

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

*Corresponding Author

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_{60} 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_2SiO_4) using global optimization with first principles energy expressions*

*Corresponding Author

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.

ACKNOWLEDGMENTS

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.

First of all, I would like to thank Alessandra Candian for supporting, inspiring, and mentoring me in the first two years of my PhD. I thank her for teaching me, not just how to do research, but also the political aspect of academia.

A special thank goes to the EuroPAH network for this beautiful experience. I am so grateful to have had this privilege. Hence, I would like to thank Liv Hornekær, Andrew Cassidy, and John Thrower for the collaborations and training that helped me develop as a scientist. I thank all EuroPAH ESRs (Early Stage Researchers): Gabi, Lindsey, Juliana, Shreyak, Martin, Sanjana, Evgeny, Georgios, Rushdi, Yaolin, Lorenzo, Laurène, Zeyuan, Rijutha, and Frederik (even though he is not an ESR, we always considered him as part of the group). From Aarhus University, I would also like to thank Bjørk Hammer for hosting me during my secondment and Wilke Dononelli for supervising my machine learning calculations.

I would like to thank all current members and past members of the interstellar medium group (the pizza meeting!) of which I have been in charge for three years: Andrew, Pedro, Kimberly, Cornelia, Marina, Morgan, Claudia, Sascha, Andrew, Pablo, Lizette, Raymond, Jordy, Ümit, Kevin and my office mates Cameron and Morgan.

I acknowledge the astrobiology group in Utrecht: Claudia, Nina, Eloi, and Alexandra as well as Helen King and the former members Vincent, Arjen, Kateryna, and Lucas. Thanks also to Nelson Dzade for his support and teachings as well as Mariëtte Wolthers, Sergio Ruiz Hernandez, and Nora de Leeuw for their input on chapter 4 and 5.

I thank Jordy for being my science buddy and forcing me to study hard every day due to his daily scientific questions.

Now, a special thank goes to Michał Bulak, a friend, colleague, and ESR fellow that was a witness of this journey and for his unconditional support and love (proverbs 17:17, "A friend loves at all times, and a brother is born for adversity").

I thank Folkert as well as Marina for supporting and advising me during a hard time in this pandemic and for correcting the dutch version of the summary of this thesis.

A big thank goes to Marta for designing the amazing cover of this thesis.

I thank all the secretaries: Monica and Marjan for the daily pleasant chat and support as well as Susan and Alexandra. I would like to thank also Els and Evelijn for helping me with the EuroPAH budget. A double thank goes to Evelijn for helping me when I was in Aarhus during the corona outbreak.

I would like to thank Gabriella for helping me to finalize the non-scientific part of this thesis as well as for the pleasant Italian chats.

I thank Dilovan for the friendly coffee break chats (pre-pandemic) in my office and for helping me to finalize my propositions.

Now, I would like to mention all the people that did not directly contributed to this thesis and I met in Leiden during this journey. I thank all my friends and colleagues: Anna, Fraser, Kirsty, Marta, Danna, Lammim, Martijn (Oei), Martijn (van Gelder), Jeroen, Alex, Patrick, Bas, Mantas, Dieuwertje, Omar, Margot, Gwén, Lydia, Pooneh, Erik, Roland, Frits, Stijn, Sarah, Helgi, Sandra, Benoit, Matus and the new PhD students (I wish I could have had more time to know you better) Roi, Elina, Tara, Niccolò, Joshua, Pranjal and Julia.

A special shazam goes to Turgay (he knows what this means) for his unmanageable sense of humor and support.

I would like to mention the people that contributed and helped me to keep going with my hobbies alongside science. I thank Anniek that pushed me to restart a hobby and passion that I stopped 12 years ago. Another special thank goes to my former band members, colleagues and friends (Dario and the Monkeys). Specifically, Łukasz (the sad monkey) for your unconditional friendship, helping me with the final steps of this thesis and trusting me with an honor of being a witness at your wedding. I am so grateful to have met you, you are the real star of this band. Hiddo (the happy monkey), thanks for your friendship and for being the happy light of this band. I thank my new band (Dario and the Guinea Pigs) specifically Alice and Evgenii (Chaikin) who helped me improve my vocal cords and supported me with some music during the lockdown. Evgenii thanks also for all the pleasant chats and friendship outside the music.

I would like to thank Carla Murineddu and the modern dance group at USC Leiden, this is a wonderful initiative that all universities should have (mens sana in corpore sano).

Finally, I acknowledge my supervisors A.G.G.M. Tielens, I.L. ten Kate, and T. Lamberts for their support and fruitful discussions.

Ringraziamenti

Ringrazio me stesso per essermi permesso tutto questo. Ringrazio la mia famiglia, in particolare, mio padre e mia madre che hanno creduto in me e supportato in questo cammino.

Ringrazio Roberta per il suo so/supporto.

Ringrazio Valeria Amaro, la prima persona italiana che conobbi a Leiden, per le risate, la sua amicizia e i nostri battibecchi scientifici.

Un ringraziamento speciale a Rocco Martinazzo per il suo supporto teorico e i suoi insegnamenti. Ringrazio anche Mirko Leccese per la sua amicizia e lo scambio di opinioni, via whatsapp, che mi ha aiutato ad aggiornare le mie conoscienze di chimica teorica.

Ringrazio Dario Duca e Remedios Cortese per il loro supporto scientifico e i loro consigli.

Ringrazio Elvira Piccione per avermi permesso di tenere un seminario al mio vecchio liceo. E' stata una grande emozione ritornare, ma dall'altro lato del banco.

Uno speciale ringraziamento a Clarissa Arvizzigno per la sua amicizia, il suo supporto morale e per avere controllato la versione italiana del riepilogo di questa tesi.