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Computational electrocatalysis: methods and fundamental applications on CO₂ reduction and formic acid oxidation

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LIST OF PUBLICATIONS, CONFERENCES AND AWARDS

Publications

Chapter 2

Granda-Marulanda, L. P., Builes, S., Koper, M. T. M. & Calle-Vallejo, F. Influence of Van der Waals Interactions on the Solvation Energies of Adsorbates at Pt-Based Electrocatalysts. *ChemPhysChem* **20**, 2968–2972 (2019).

Chapter 3

Granda-Marulanda, L. P., McCrum, I. T. & Koper, M. T. M. A simple method to calculate solution-phase free energies of charged species in computational electrocatalysis. *J. Phys.: Condens. Matter* **33**, 204001 (2021).

Chapter 4

Granda-Marulanda, L. P., Builes, S., Koper, M. T. M., Illas, F. & Calle-Vallejo, F. A Semiempirical Method to Detect and Correct DFT-Based Gas-Phase Errors and Its Application in Electrocatalysis. *ACS Catal.* **10**, 6900–6907 (2020).

Chapter 5

Chen, X., **Granda-Marulanda, L. P.**, McCrum, I. T. & Koper, M. T. M. Adsorption processes on a Pd monolayer-modified Pt(111) electrode. *Chem. Sci.* **11**, 1703–1713 (2020).

Chapter 6

Chen, X., **Granda-Marulanda, L. P.**, McCrum, I. T. & Koper, M. T. M. How Palladium prohibits CO poisoning during electrocatalytic formic acid oxidation and carbon dioxide reduction. (2021). *Submitted*

Conferences

69th Annual Meeting of the International Society of Electrochemistry

Electrochemistry from Knowledge to Innovation, 2 to 7 September 2018. Bologna, Italy
Laura Granda Marulanda, Xiaoting Chen, Ian McCrum, Federico Calle-Vallejo, Marc Koper. Insights into HCOOH Oxidation and HCOOH Production from CO₂ on Pd_{ML}/Pt-based Electrocatalysts from Theoretical and Experimental Studies. [poster]

Awards

HPC-Europa3 Transnational Access programme -2019

A scholarship to promote collaborations within the theoretical/computational scientific community within Europe. Awarded with computing time in the MareNostrum super computer in Barcelona. Hosted by Dr. Federico Calle-Vallejo of the Institute of Theoretical and Computational Chemistry of the Universitat de Barcelona (IQTUB)

ISE poster prize -2018

Poster prize at the 69th Annual Meeting of the International Society of Electrochemistry in Bologna, Italy.



Academiegebouw van de Universiteit Leiden
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I remember very well the sunny day in September 2016 when I came to Leiden for my interview. I had missed the bus stop to the university and ended up a few blocks away. I was panicking because I got lost, but I finally made it to the interview. Finishing my PhD is just the beginning of a new chapter, but it is also the closure of a 12-year chapter of my life. It started when I enrolled the graduate program at Texas A&M back in 2009, then I took a longer path, but that allowed me to see the other side of the world (literally), a world I never imagined I will live in. This opportunity made me grew on a personal and professional level and allowed me to finish my graduate studies.

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CURRICULUM VITAE

Laura Patricia Granda Marulanda was born on 9th June 1988 in Cali, Colombia. At the age of 6 she moved to Puerto Rico where she completed her high school and bachelor education. She enrolled the Chemistry program from the university of Puerto Rico at Mayagüez graduating in 2009. During this period, she did an internship at the university of Minnesota in the USA under the LANDO program and worked on the project "Design of a solid-contact ion selective electrode for the detection of perfluoroalkyl acids". From 2009 to 2011 she enrolled graduate studies and worked as a teacher assistant in the Chemistry department at Texas A&M. There, her preliminary research involved fundamental studies of silicate minerals using the Atomic Force Microscope. Later, fascinated by the world of computational chemistry, she redirected her research interests and enrolled the faculty of Physical Chemistry at the University of Belgrade in Serbia, where she completed her master's degree in 2013 on the project: "Theoretical study of the interaction of PtTM dimers (TM = Ru, Rh, Pd, Ir and Pt) with MgO(001) surface - adsorption, mobility and electronic structure".

In January 2017, Laura started her PhD in the CASC group, Leiden University, The Netherlands under the supervision of prof. dr. M. T. M. Koper. The main results obtained during this graduate research are described in this thesis, presented at international conferences and published in scientific journals.

Besides science, Laura enjoys long walks, dancing salsa and bachata, doing Zumba®, pole fitness, and loves to gaze at the horizon. She used to play the oboe, and now she is learning the ukulele. She also enjoys listening to informative podcasts and reading.