Ageo Meier de Andrade

Curriculum Vitae

About me

I am a postdoctoral researcher at Chalmers University of Technology with experience in atomistic first-principles modelling methods. My research interests comprise complex materials and interfaces investigated at the atomistic level with the help of efficient algorithms and machine learning models. As a main or co-investigator, I conducted modelling in various high-performance computers from the Swedish National Infrastructure of Computing and independently described the main findings in peer-review publications. As a lab teacher, I contributed to various bachelor's and master's level courses at Uppsala University, supporting the students and improving lab materials and environments.

Employment

2021-Current **Postdoctoral researcher**, *Department of Chemistry and Chemical Engineering*, Chalmers University of Technology, Gothenburg, Sweden.
I develop mechanistic insights into sensitisation processes caused by the entry of hydrogen in Ni-base alloys.

2017-2021 **PhD. student**, *Department of Chemistry - Ångström Laboratory*, Uppsala University, Uppsala, Sweden.
My research focused on the theoretical aspect of catalysts by means of Density Functional Theory calculations.

Education

2021 **Doctor of Philosophy. Chemistry with specialisation in Materials Chemistry**, Uppsala University, Uppsala, Sweden.
Thesis: Transition metal and alloy catalysts in the light of computational materials modelling.
Supervisor: Peter Broqvist

2020 **Licentiate of Philosophy. Chemistry with specialisation in Materials Chemistry**, *Uppsala University*, Uppsala, Sweden.
Thesis: Modeling catalysts for a sustainable future: On the importance of dispersion interactions when deciphering molecule-surface interactions.
Supervisor: Peter Broqvist

2016 **Master's degree in Applied Chemistry**, *State University of Ponta Grossa*, Ponta Grossa, Brazil.
Dissertation title: Molecular and electronic structure simulations of conductive polymers
Supervisor: Sergio Ricardo de Lazaro

Chalmers university of Technology – Gothenburg, Sweden
✉ *ageo@chalmers.se*

2013 **Bachelor's degree in Chemical Technology with an emphasis in Environmental Chemistry**, *State University of Ponta Grossa*, Ponta Grossa, Brazil.

Complementary Courses

2018 **Advanced first principles simulation**, *CCP5 Summer school, Lancaster University*, Lancaster, United Kingdom.

2015 **Workshop on Advanced Functionalities in Density Functional Theory Calculations**, *University of Sao Paulo*, Sao Paulo, Brazil.

2012 **Materials Modeling School**, *Sao Paulo State University*, Bauru, Brazil.

Experience

Laboratory teacher

2017–2021 **Computational Quantum Chemistry for Molecules and Materials**, *Uppsala University*, Uppsala, Sweden.
Course responsible: Kersti Hermansson (2017) and Chao Zhang (2018 - 2021)

2017–2021 **Chemical Bonding and Quantum Chemistry**, *Uppsala University*, Uppsala, Sweden.
Course responsible: Kersti Hermansson (2017) and Chao Zhang (2018 - 2021).

2017–2021 **Theoretical Chemistry**, *Uppsala University*, Uppsala, Sweden.
Course responsible: Roland Lindh.

2017–2021 **Materials Modelling**, *Uppsala University*, Uppsala, Sweden.
Course responsible: Jolla Kullgren.

2020–2021 **Quantum mechanics and chemical bonding I**, *Uppsala University*, Uppsala, Sweden.
Course responsible: Nessima Sahli.

2021 **Theoretical Chemistry - profile course**, *Uppsala University*, Uppsala, Sweden.
Course responsible: Peter Broqvist.

2020 **Quantum mechanics and chemical bonding II**, *Uppsala University*, Uppsala, Sweden.
Course responsible: Nessima Sahli.

Academic research

2016/04–2016/06 **Assistant research**, *Structural and Electronic Investigation of Cu bulk and Cu_2O by SCC-DFTB Calculations*, Uppsala University, Uppsala, Sweden.
Leader: Peter Broqvist.

2012-2013 **Research trainee**, *Theoretical study, by DFT methodologies, of the tin tartrate electronic structure*, State University of Ponta Grossa, Paraná, Brazil.
Leader: Alexandre Camilo Junior.

2011-2012 **Research trainee**, *Theoretical study of the tin tartrate electronic structure*, State University of Ponta Grossa, Paraná, Brazil.
Leader: Alexandre Camilo Junior.

2010-2011 **Research trainee**, *Conformers of N,N-dialyl-2,2-dichloracetamide herbicide*, State University of Ponta Grossa, Paraná, Brazil.
Leader: Barbara Celania Fiorin.

Awards

2020 **Liljewalch travel scholarship**, *Holding period: VT20-VT20*.

2019 **Liljewalch travel scholarship**, *Holding period: VT19-VT19*.

2018 **Best Poster**, *Awarded to the second prize*, CCP5 Summer School.

Computer skills

Computational Chemsitry softwares

Advanced
Cambridge serial total energy package (CASTEP)
Vienna ab-initio simulation package (VASP)
Atomic simulation environment (ASE)
DFTB+
Gaussian09
General atomic and molecular electronic structure system (GAMESS)
Molecular orbital package (MOPAC)

Intermediate
BIOVIA Materials Studio
Quantum Espresso
Crystal09

Basic
CP2K
LAMMPS molecular dynamics simulator

Programming languages

Advanced
Bash
Python

Intermediate
awk

Basic
Rust

Database query languages

Advanced
ASE

Basic
MongoDB (non-relational)
Structured query languages (PostgreSQL, MySQL)

Miscellaneous

Advanced
LaTeX

Languages

Mothertongue **Portuguese**

Advanced **English**

Intermediate **Swedish** *Capable of speak, read, listen and write*
Spanish

Interests

Professional

- Theoretical investigation of advanced materials and interfaces
- Development of workflows for high-throughput methods in Computational Chemistry

Personal

- Be proficient in other languages
- Playing guitar
- Cooking
- Traveling

References - Contact Information

Itai Panas.
E-mail address: itai.panas@chalmers.se