Vinícius Wilian D. Cruzeiro

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Research field: Computational chemistry
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EDUCATION AND TRAINING

STANFORD UNIVERSITY — Stanford, CA, USA
Postdoctoral research — Aug/2021 – Current
Advisor: Todd J. Martínez
Research: 1) Using TeraChem as an external library for faster QM/MM simulations with Amber; 2) Polarizable QM/MM simulations with TeraChem and Tinker; 3) Employing accurate post-hartree fock methods to study the x-ray emission spectrum of liquid water.

UNIVERSITY OF CALIFORNIA, SAN DIEGO — San Diego, CA, USA
Postdoctoral research — May/2019 – Aug/2021
Advisors: Andreas Götz and Francesco Paesani
Research: 1) Highly accurate many-body potentials for relevant simulations in atmospheric chemistry; 2) Theoretical description of the spectral splitting in the x-ray emission spectrum of liquid water; 3) Improvements in the *ab initio* electronic structure software Quick, including QM/MM simulations in Amber

UNIVERSITY OF FLORIDA — Gainesville, FL, USA
Doctoral degree in chemistry — Aug/2014 – May/2019
Advisor: Adrian Roitberg
Research: Efficient constant pH and redox potential molecular dynamics with multidimensional replica exchange simulations
GPA: 4.0/4.0

UNIVERSITY OF SAO PAULO — São Paulo, SP, Brazil
Master's degree in physics — Jan/2012 – Mar/2014
Advisor: Kaline Coutinho
Research: Thermal effects on the gas-phase absorption spectrum of photosynthetic pigments using classical and *ab initio* molecular dynamics
GPA: 4.0/4.0

FEDERAL UNIVERSITY OF GOIAS — Goiânia, GO, Brazil
Bachelor's degree in physics — Jan/2008 – Dec/2011
Advisor: Herbert Georg
Research: Applying the electrostatically embedded many-body expansion for faster and accurate *ab initio* molecular dynamics
GPA: 4.0/4.0

PUBLICATIONS

Under review or in preparation

19) **Cruzeiro, V.W.D.;** Wang, Y.; Pieri, E.; Hohenstein, E.G.; Martínez, T.J.; TCPB: accessing TeraChem as an external library for faster QM or QM/MM simulations. (Manuscript available upon request)

Peer-reviewed

18) **Cruzeiro, V.W.D.;** Galib, M.; Limmer, D.T.; Götz, A.; Insights into the uptake of N_2O_5 by aqueous aerosol using chemically accurate many-body potentials. *Nature Commun.*, 13: 1266 (2022). *(• Highlighted with a press release)*

17) Ahn, S.; Seitz, C.; **Cruzeiro, V.W.D.;** McCammon, J.A.; Götz, A.; Data for molecular dynamics simulations of escherichia coli cytochrome bd oxidase with the amber force field. *Data Brief*, 38: 107401 (2021).

16) **Cruzeiro, V.W.D.;** Wildman, A.; Li, X.; Paesani, F.; Relationship between hydrogen-bonding motifs and the $1b_1$ splitting in the x-ray emission spectrum of liquid water. *J. Phys. Chem. Lett.*, 12: 3996 (2021).

15) **Cruzeiro, V.W.D.;** Lambros, E.; Riera, M.; Roy, R.; Paesani, F.; Götz, A.; Highly accurate many-body potentials for simulations of N_2O_5 in water: benchmarks, development, and validation. *J. Chem. Theory Comput.*, 17: 3931 (2021). (• *Front cover of the journal)*

14) **Cruzeiro, V.W.D.;** Manathunga, M.; Merz, K.M.; Götz, A.; Open-Source Multi-GPU-Accelerated QM/MM Simulations with AMBER and QUICK. *J. Chem. Inf. Model*, 61: 2019 (2021). *(• Highlighted with a press release)*

13) Manathunga, M.; Jin, C.; **Cruzeiro, V.W.D.;** Miao, Y.; Mu, D.; Arumugam, K.; Keipert, K.; Aktulga, H.M.; Merz, K.M.; Götz, A.; Harnessing the Power of Multi-GPU Acceleration into the Quantum Interaction Computational Kernel Program. *J. Chem. Theory Comput.*, 17: 3955 (2021). *(• Highlighted with a press release)*

12) Bueno, P.; **Cruzeiro, V.W.D.;** Roitberg, A.; Feliciano, G.; The density-of-states and equilibrium charge dynamics of redox-active switches. *Electrochim. Acta*, 387: 138410 (2021).

11) **Cruzeiro, V.W.D.;** Feliciano, G.T.; Roitberg, A.E.; Exploring coupled redox and pH processes with computational chemistry: applications to five different systems. *J. Am. Chem. Soc.*, 142: 3823 (2020). *(• Highlighted in JACS Spotlights)*

10) **Cruzeiro, V.W.D.;** Gao, X.; Kleiman, V.D.; Implementing new educational platforms in the classroom: an interactive approach to the particle in a box problem. *J. Chem. Educ.*, 96: 1663 (2019).

9) **Cruzeiro, V.W.D.;** Roitberg, A.E.; Multidimensional replica exchange simulations for efficient constant pH and redox potential molecular dynamics. *J. Chem. Theory Comput.*, 15: 871 (2019).

8) **Cruzeiro, V.W.D.;** Amaral, M.S.; Roitberg, A.E.; Redox potential replica exchange molecular dynamics at constant pH in Amber: Implementation and validation. *J. Chem. Phys.*, 149: 072338 (2018). *(• Front cover of the journal. • 2018 JCP Editors' Choice article. • Featured paper. • Highlighted with a press release)*

7) Bell, M.R.; **Cruzeiro, V.W.D.;** Cismesia, A.P.; Tesler, L.F.; Roitberg, A.E.; Polfer, N.C.; Probing the structures of solvent-complexed ions formed in electrospray ionization using cryogenic infrared photodissociation spectroscopy. *J. Phys. Chem. A*, 122: 7427 (2018).

6) Chouinard, C.D.; **Cruzeiro, V.W.D.;** Kemperman, R.H.J; Oranzi, N.R.; Roitberg, A.E.; Yost, R.A.; Cation-dependent conformations in 25-hydroxyvitamin D3-cation adducts measured by ion mobility-mass spectrometry and theoretical modeling. *Inter. J. Mass Spectrom.*, 432: 1 (2018).

5) Chouinard, C.D.; **Cruzeiro, V.W.D.;** Roitberg, A.E.; Yost, R.A.; Experimental and theoretical investigation of sodiated multimers of steroid epimers with ion mobility-mass spectrometry. *J. Am. Soc. Mass Spectrom.*, 28: 323 (2017).

4) Chouinard, C.D.; **Cruzeiro, V.W.D.;** Beekman, C.R.; Roitberg, A.E.; Yost, R.A.; Investigating differences in gas-phase conformations of 25-hydroxyvitamin D3 sodiated epimers using ion mobility-mass spectrometry and theoretical modeling. *J. Am. Soc. Mass Spectrom.*, 28: 1497 (2017).

3) **Cruzeiro, V.W.D.;** Roitberg, A.E.; Polfer, N.C.; Interactively Applying the variational method to the dihydrogen molecule: exploring bonding and antibonding. *J. Chem. Educ.*, 93: 1578 (2016).

2) Bhatt, A.; Mahon, B.P.; **Cruzeiro, V.W.D.;** Cornelio, B.; Laronze-Cochard, M.; Ceruso, M.; Sapi, J.; Rance, G.A.; Khlobystov, A.N.; Fontana, A.; Roitberg, A.; Supuran, C.T.; McKenna, R.; Structure activity relationships of benzenesulfonamide-based inhibitors towards carbonic anhydrase isoform specificity. *Chembiochem*, 18: 213 (2016).

1) Cabral, B.J.C.; **Cruzeiro, V.W.D.;** Coutinho, K.; Canuto, S; Free base phthalocyanine: influence of thermal effects and dimerization on the electronic absorption spectrum. *Chem. Phys. Let.*, 595: 97 (2014).

AWARDS AND HONORS (‡ Top 3 awards)

13) ‡ *Wiley Computers in Chemistry Outstanding Postdoc award*, American Chemical Society (2022).

12) Selected for *NextProf Science*, University of Michigan (2021).

11) Winner of *Outstanding Lightning Talk competition*, Virtual Conference in Theoretical Chemistry, Stanford University (2020).

10) Selected for *Building Future Faculty Program*, North Carolina State University (2020).

9) ‡ *NVIDIA GPU award*, American Chemical Society (2019).

8) *MolSSI travel award*, The Molecular Sciences Software Institute (2019).

7) ‡ *Chemical Computing Group excellence award for graduate students*, American Chemical Society (2018).

6) *Early career physical chemistry award*, University of Florida (2015).

5) *Townes R. Leigh award*, University of Florida (2015).

4) *Grinter fellowship*, University of Florida (2014).

3) *Graduate fellowship* for studies at the University of Florida, CAPES, Brazil (2014-2018).

2) *Graduate fellowship* for studies at the University of São Paulo, CNPq, Brazil (2012-2014).

1) *Undergraduate research scholarship*, CNPq, Brazil (2009-2011).

RESEARCH EXPERIENCE

STANFORD UNIVERSITY, Postdoctoral research Stanford, CA, USA
Advisor: Todd J. Martínez Aug/2021 – Current

- Allowed access to TeraChem as an external library and applied this implementation for faster QM/MM simulations in Amber.
- Building upon previous research at UCSD, employed accurate multireference post-hartree fock methods, namely EOM-IP-CCSD and SA-CASSCF, to study the x-ray emission spectrum of liquid water. Also assessed how core-hole dynamical effects influence the spectrum.
- Worked on an interface between TeraChem and Tinker for polarizable QM/MM simulations.
- Employed all QM and QM/MM calculations to study a classic enzymatic catalyzed reaction: nucleophilic attack on serine proteases.

UNIVERSITY OF CALIFORNIA, SAN DIEGO, Postdoctoral research San Diego, CA, USA
Advisor: Andreas Götz May/2019 – Aug/2021

Main project:

- Employed accurate fitting approaches and fragmentation methods to generate potentials with CCSD(T) accuracy for molecular simulations of clusters, interfaces, and bulk.
- The new potentials follow the same characteristics of the highly successful MB-pol water model, which combines a physically motivated representation of long-range interactions with accurate low-order terms of the many-body expansion. MB-pol accurately describes experimental properties of water across different phases.
- Newly generated potentials were used in simulations of dinitrogen pentoxide (N_2O_5) in water, which are relevant in atmospheric chemistry because N_2O_5 is an important intermediate in reactions of nitrogen oxides related to air quality and climate. This project was part of the Center for Aerosol Impacts on Chemistry of the Environment (CAICE), an NSF funded institution with 26 experimental and theoretical groups.

Other contributions:

- Performance improvements in one electron integrals at the *ab initio* quantum chemistry software Quick.
- Implemented in Sander (MD engine from Amber) an interface to Quick which allows QM/MM simulations with multi-GPU-acceleration. Since Quick and Sander are open-source, these simulations can be performed free of charge.
- Computed Amber force field parameters for heme b_{558}, heme b_{595}, and heme d, enabling simulations of *Escherichia coli* cytochrome *bd* oxidase and related systems.

Advisor: Francesco Paesani May/2019 – Aug/2021

Main project:

- Investigated the x-ray emission spectrum of liquid water that exhibits a spectral split in the $1b_1$ region associated with the hydrogen-bonding environment. Despite previous theoretical and experimental research on this feature, the causes that give rise to the splitting were not yet definitively identified.
- Made use of path integral molecular dynamics (PIMD) with the MB-pol model. These simulations accurately describe water across different phases and contain quantum nuclei effects.
- Performed TD-DFT calculations aiming at high-energy emissions for the study of the split spectral feature.
- Provided novel insights from a theoretical perspective about the different hypotheses in the literature that attempt to describe the origin of this spectrum feature. Showed the relation between the different hydrogen-bonding motifs and the theoretical x-ray emission spectrum.

Other contributions:

- Exploited how many-body effects are described by deep neural networks.

UNIVERSITY OF FLORIDA, Doctoral degree in chemistry Gainesville, FL, USA

Advisor: Adrian Roitberg Aug/2014 – May/2019

Main project:

- Developed, tested, validated, and implemented in Amber new methods that allow the theoretical study of electrochemical processes through simulations at constant redox potential and pH.
- Implemented in Amber new replica exchange techniques that allow converged results to be obtained more efficiently.
- All these new Amber implementations are available using GPU-accelerated code, which provides high-performance to the simulations. These are the first implementations of constant redox potential methods in a common molecular dynamics package.

Other contributions:

- Collaborated with different experimental groups by applying computational chemistry to aid in explaining a variety of problems, like different epimer conformers in Ion Mobility-Mass Spectrometry experiments, inhibitor functionality in cancer drug targets, and conformations of solvent-tagged ions in infrared photodissociation spectroscopy experiments.

UNIVERSITY OF SAO PAULO, Master's degree in physics São Paulo, SP, Brazil

Advisor: Kaline Coutinho Jan/2012 – Mar/2014

- Studied thermal effects on the gas-phase electronic absorption spectrum of monomers and dimers of different porphyrins and phthalocyanines. Classical and *ab initio* molecular dynamics were employed.
- Proposed a new set of force field parameters to reproduce better the conformations yielded by *ab initio* molecular dynamics.
- Performed experimental measures of the absorption spectra of phthalocyanines as a function of pH.

FEDERAL UNIVERSITY OF GOIAS, Bachelor's degree in physics Goiânia, GO, Brazil

Advisor: Herbert Georg Jan/2009 – Dec/2011

- Applied the many-body expansion as an approach to significantly speedup *ab initio* molecular dynamics simulations without significant loss in accuracy. This methodology has been employed to reproduce post-HF calculations.
- Implemented a software to perform many-body expansion and molecular dynamics calculations. Electronic structure calculations are performed on an external software.

MOST RELEVANT CONFERENCE PRESENTATIONS (Out of a total of 30)

Cruzeiro, V.W.D.; Paesani, F.; Theoretical description of the $1b_1$ splitting in the x-ray emission spectrum of liquid water. **Oral presentation;** Virtual Conference in Theoretical Chemistry, Online, Stanford University (2020). (• *Presented as a featured speaker for winning Outstanding Lightning Talk competition*)

Cruzeiro, V.W.D.; Possible applications for the open molecular science cloud: Amber simulations and development of highly accurate many-body potentials. **Oral presentation;** 12th European Conference on Computational and Theoretical Chemistry, Perugia and Rome, Italy (2019).

Cruzeiro, V.W.D.; Roitberg, A.E.; GPU-accelerated constant pH and redox potential molecular dynamics: exploring electrochemistry in Amber. **Sci-Mix and COMP poster presentation;** 257th ACS National Meeting and Exposition, San Diego, CA, USA (2019).

Cruzeiro, V.W.D.; Roitberg, A.E.; Efficient constant pH and redox potential molecular dynamics with multidimensional replica exchange simulations. **Sci-Mix and COMP poster presentation;** 256th ACS National Meeting and Exposition, Boston, MA, USA (2018).

Cruzeiro, V.W.D.; Roitberg, A.E.; High-performance multidimensional replica exchange molecular dynamics along pH, redox potential and temperature dimensions using Amber. **Sci-Mix and COMP poster presentation;** 255th ACS National Meeting and Exposition, New Orleans, LA, USA (2018).

Cruzeiro, V.W.D.; Roitberg, A.E.; Applying theoretical modeling to help the interpretation of ion mobility/mass spectrometry experiments: the case of cation-dependent 25-hydroxyvitamin D3 conformations. **Oral and poster presentation;** ASMS Sanibel Conference, St. Petersburg, FL, USA (2018).

Cruzeiro, V.W.D.; Amaral, M.S.; Roitberg, A.E.; High-performance molecular dynamics at constant pH and constant redox potential using Amber. **Oral presentation;** 253rd ACS National Meeting and Exposition, San Francisco, CA, USA (2017).

Cruzeiro, V.W.D.; Roitberg, A.E.; Applying theoretical modeling to help the interpretation of ion mobility/mass spectrometry experiments. **Oral presentation;** 91st Florida Annual Meeting and Exposition (FAME), Tampa, FL, USA (2016).

Cruzeiro, V.W.D.; Georg, H.C.; Applying the many-body expansion for *ab initio* molecular dynamics. **Oral presentation;** II Brazilian School of Molecular Modeling, Santo André, Brazil (2013).

Cruzeiro, V.W.D.; Coutinho, K.; Cabral, B.J.C.; Canuto, S.; Theoretical study of the absorption spectra of photosynthetic pigments. **Poster presentation;** Workshop on Biomolecular Theory-Experiment Interplay, São Paulo, Brazil (2013).

ACADEMIC SERVICE, LEADERSHIP AND MENTORING EXPERIENCE

Served as a journal reviewer: 1) The Journal of Physical Chemistry; 2) Journal of Chemical Theory and Computation; 3) Journal of Chemical Education; 4) Journal of Molecular Liquids; 5) Spectrochimica Acta Part A.

Co-organized symposium for the ACS Fall 2022 meeting, "A symposium in honor of the 60th birthday of prof. Adrian Roitberg" at Chicago, IL. Aug/2022.

Protein subgroup leader, Martínez group at Stanford University. Oct/2021 – Current.

Served as a computational chemistry judge on LatinXChem, online. Sep/2021 and Sep/2022.

Mentoring experience (2 graduate students), Martínez group at Stanford University. Aug/2021 – Current.

Mentoring experience (1 graduate student and 1 undergraduate student), Paesani group at University of California, San Diego. May/2019 – Aug/2021.

Letters to a Pre-Scientist
Role: Scientist Pen Pal Aug/2018 – Current

- This program connects students from high-poverty schools with real scientists. The idea is that this connection can help with students' education. From this "scientific interaction", that most students likely would not have otherwise, they may be encouraged to afterwards follow a STEM career.

COMPUTATIONAL SKILLS

Languages: Fortran, Python, Bash/Shell, C++, CUDA, MPI, OpenMP, PHP, HTML, SQL.
Experience: Amber developer (since 2017), TeraChem developer (since 2021), parallel programming, object-oriented programming, server management, web development.
Contributions to Amber (popular software for molecular simulations): 1) Constant pH and redox potential molecular dynamics in both implicit and explicit solvent; 2) Redox potential replica exchange molecular dynamics; 3) Multi-dimensional replica exchange support for pH and redox potential dimensions; 4) Novel interface for fast QM/MM simulations with TeraChem; 5) Implemented an interface with Quick that allows multi-

GPU-accelerated QM/MM simulations; 6) Implementation of new AmberTools for preparation of input files and analyses of output files; 7) Several bug fixes.
Contributions to TeraChem (software for electronic structure calculations): 1) Allow TeraChem to be used as an external library using a client/server model and Google's protocol buffers; 2) Place a continuous integration and continuous delivery (CI/CD) platform using GitHub Actions; 3) Several bug fixes.

TEACHING EXPERIENCE

UNIVERSITY OF FLORIDA Gainesville, FL, USA
Graduate Teaching Assistant Aug/2014 – May/2019

- Development of educational interactive platforms that allow students to better explore the class material. (See publications in the *J. Chem. Educ.*)
- Graduate courses taught:
    - CHM6586 - Computational Chemistry. Description: this course is offered to students from different departments that have different backgrounds. The students gain practical experience (on how to choose a good combination of method/basis set, how to perform basis set extrapolation, etc.) as well as a theoretical basis behind common algorithms (as self-consistent field, geometry optimization, and frequency calculations) and methods (like Hartree-Fock, MP2, and DFT) in electronic structure software.
    - CHM6470 - Chemical Bond & Spectra 1. Description: in this course, students learn quantum mechanics, with a focus in theoretical chemistry.
- Undergraduate courses taught:
    - CHM4411 - Physical Chemistry
    - CHM3400 - Physical Chemistry with Applications to Biology

UNIVERSITY OF SAO PAULO São Paulo, SP, Brazil
Teaching Assistant Jan/2012 – Mar/2014

- Undergraduate courses taught:
    - Physics I
    - Introduction to Physics

FEDERAL UNIVERSITY OF GOIAS Goiânia, GO, Brazil
Teaching Assistant Jan/2009 – Dec/2011

- Undergraduate courses taught:
    - Physics I
    - Physics II

LANGUAGES

Portuguese. Mother tongue.

English. Fluent in speech, writing and reading.

Spanish. Fluent in speech and reading. Intermediate in writing.