Stanford

Vinícius Wilian D. Cruzeiro

Postdoctoral Scholar, Chemistry

Bio

BIO

Vinícius Cruzeiro explores computational/theoretical chemistry aiming at accurately describing the behavior of proteins, biomolecules, and related systems using molecular simulations, quantum mechanics, and machine learning representations. This research digs into fundamental aspects of nature at the intersection of physics, chemistry, and biology. The knowledge gained is employed to complement experiments (that cannot achieve atomic detail) and can drive the design of new materials and pharmaceutical applications, such as in drug discovery. Dr. Cruzeiro actively collaborates with experimentalists and other theoretical researchers.

Dr. Cruzeiro is part of the Amber developer's team. He has participated in developing different methodologies, including molecular simulations with coupled electrochemical and pH effects, enhanced sampling techniques, and quantum mechanics/molecular mechanics approaches. Amber is a popular software package for molecular simulations used by several research groups worldwide.

HONORS AND AWARDS

- NVIDIA GPU award, American Chemical Society (2019)
- Chemical Computing Group excellence award for graduate students, American Chemical Society (2018)
- MolSSI travel award, The Molecular Sciences Software Institute (2019)
- Townes R. Leigh award, University of Florida (2015)
- Early career physical chemistry award, University of Florida (2015)
- Grinter fellowship, University of Florida (2014)
- Graduate fellowship for studies at the University of Florida, CAPES, Brazil (2014-2018)
- NextProf Science, University of Michigan (2021)
- Building Future Faculty Program, North Carolina State University (2020)
- Graduate fellowship for studies at the University of São Paulo, CNPq, Brazil (2012-2014)
- Undergraduate research scholarship, CNPq, Brazil (2009-2011)

PROFESSIONAL EDUCATION

- Postdoc, University of California, San Diego (2021)
- Doctor of Philosophy, University of Florida (2019)
- Master of Science, University of Sao Paulo (2014)
- Bachelor of Science, Universidade Federal De Goias (2011)

STANFORD ADVISORS

- Todd Martinez, Postdoctoral Faculty Sponsor

LINKS

- Google Scholar: https://scholar.google.com/citations?user=iAK04WMAAAAJ&hl=en
- Twitter: https://twitter.com/vwcruzeiro

Publications

PUBLICATIONS

- **Harnessing the Power of Multi-GPU Acceleration into the Quantum Interaction Computational Kernel Program** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Manathunga, M., Jin, C., Cruzeiro, V. D., Miao, Y., Mu, D., Arumugam, K., Keipert, K., Aktulga, H., Merz, K. M., Goetz, A. W.
  2021; 17 (7): 3955-3966

- **Highly Accurate Many-Body Potentials for Simulations of N2O5 in Water: Benchmarks, Development, and Validation** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Cruzeiro, V. D., Lambros, E., Riera, M., Roy, R., Paesani, F., Gotz, A. W.
  2021; 17 (7): 3931-3945

- **Open-Source Multi-GPU-Accelerated QM/MM Simulations with AMBER and QUICK** *JOURNAL OF CHEMICAL INFORMATION AND MODELING*
  Cruzeiro, V. D., Manathunga, M., Merz, K. M., Gotz, A. W.
  2021; 61 (5): 2109-2115

- **Relationship between Hydrogen-Bonding Motifs and the 1b(1) Splitting in the X-ray Emission Spectrum of Liquid Water** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Cruzeiro, V. D., Wildman, A., Li, X., Paesani, F.
  2021; 12 (16): 3996-4002

- **The density-of-States and equilibrium charge dynamics of redox-active switches** *Electrochimica Acta*
  Bueno, P. R., Cruzeiro, V. D., Roitberg, A. E., Feliciano, G. T.
  2021; 387: 138410

- **Exploring Coupled Redox and pH Processes with a Force-Field-Based Approach: Applications to Five Different Systems** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Cruzeiro, V. D., Feliciano, G., Roitberg, A. E.
  2020; 142 (8): 3823-3835

- **Implementing New Educational Platforms in the Classroom: An Interactive Approach to the Particle in a Box Problem** *JOURNAL OF CHEMICAL EDUCATION*
  Cruzeiro, V. D., Gao, X., Kleiman, V. D.
  2019; 96 (8): 1663-1670

- **Multidimensional Replica Exchange Simulations for Efficient Constant pH and Redox Potential Molecular Dynamics** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
  Cruzeiro, V. D., Roitberg, A. E.
  2019; 15 (2): 871-881

- **Probing the Structures of Solvent-Complexed Ions Formed in Electrospray Ionization Using Cryogenic Infrared Photodissociation Spectroscopy** *JOURNAL OF PHYSICAL CHEMISTRY A*
  Bell, M. R., Cruzeiro, V. D., Cismesia, A. P., Tesler, L. F., Roitberg, A. E., Polfer, N. C.
  2018; 122 (37): 7427-7436

- **Cation-dependent conformations in 25-hydroxyvitamin D3-cation adducts measured by ion mobility-mass spectrometry and theoretical modeling** *INTERNATIONAL JOURNAL OF MASS SPECTROMETRY*
  Chouinard, C. D., Cruzeiro, V. D., Kemperman, R. J., Oranzi, N. R., Roitberg, A. E., Yost, R. A.
  2018; 432: 1-8

- **Redox potential replica exchange molecular dynamics at constant pH in AMBER: implementation and validation** *JOURNAL OF CHEMICAL PHYSICS*
  Cruzeiro, V. D., Amaral, M. S., Roitberg, A. E.
  2018; 149 (7): 072338

- **Investigating Differences in Gas-Phase Conformations of 25-Hydroxyvitamin D3 Sodiated Epimers using Ion Mobility-Mass Spectrometry and Theoretical Modeling** *JOURNAL OF THE AMERICAN SOCIETY FOR MASS SPECTROMETRY*
  Chouinard, C. D., Cruzeiro, V. D., Beekman, C. R., Roitberg, A. E., Yost, R. A.
  2017; 28 (8): 1497-1505

- **Experimental and Theoretical Investigation of Sodiated Multimers of Steroid Epimers with Ion Mobility-Mass Spectrometry** *JOURNAL OF THE AMERICAN SOCIETY FOR MASS SPECTROMETRY*
  Chouinard, C. D., Cruzeiro, V. D., Roitberg, A. E., Yost, R. A.
  2017; 28 (2): 323-331

- **Structure-Activity Relationships of Benzenesulfonamide-Based Inhibitors towards Carbonic Anhydrase Isoform Specificity** *CHEMBIOCHEM*
  Bhatt, A., Mahon, B. P., Cruzeiro, V. D., Cornelio, B., Laronze-Cochard, M., Ceruso, M., Sapi, J., Rance, G. A., Khlobystov, A. N., Fontana, A., Roitberg, A., Supuran, C. T., McKenna, et al
  2017; 18 (2): 213-222

- **Interactively Applying the Variational Method to the Dihydrogen Molecule: Exploring Bonding and Antibonding** *JOURNAL OF CHEMICAL EDUCATION*
  Cruzeiro, V. D., Roitberg, A., Polfer, N. C.
  2016; 93 (9): 1578-1585

- **Free base phthalocyanine: Influence of thermal effects and dimerization on the electronic absorption spectrum** *CHEMICAL PHYSICS LETTERS*
  Cabral, B. C., Cruzeiro, V. D., Coutinho, K., Canuto, S.
  2014; 595: 97-102