

## INDEPENDENT CAREER

**Carnegie Mellon University (CMU)**

Pittsburgh, PA, USA

- Assistant Professor, Department of Chemistry & Department of Chemical Engineering
- Research program areas:  
Catalysis & Reaction Design | Artificial Intelligence & Computer Science for Chemistry |  
Organic Materials | Automated Chemical Synthesis | Physical Organic Chemistry

starting January 2022

## EDUCATION &amp; TRAINING

**University of Toronto (UofT)**, Departments of Chemistry and Computer Science

Toronto, ON, Canada

- NSERC Banting Postdoctoral Fellow
  - Project titled: “*Designing Catalysts with Artificial Intelligence*”
- Postdoctoral Research Fellow, Advisor: Professor Alán Aspuru-Guzik
  - *Visiting scholar at Vector Institute for Artificial Intelligence*
  - Developed platforms for inverse-designing catalysts with artificial intelligence
  - Provided key structural and mechanistic insights to various challenges in organic chemistry with computational methods

2020 – 2021

2019 – 2021

2019 – 2021

**Florida State University (FSU)**, Department of Chemistry and Biochemistry

Tallahassee, FL, USA

- Ph.D. in Chemistry, GPA 4.0, Advisor: Professor Igor V. Alabugin
- *in-flight* M.Sc. in Chemistry
- Ph.D. Dissertation entitled: “*Controlling Chemical Reactivity with Stereoelectronic Effects*”

2014 – 2018

2014 – 2016

**Federal University of Rio de Janeiro (UFRJ)**, Institute of Chemistry

Rio de Janeiro, RJ, Brazil

- B.Sc. in Chemistry, with technological attributions, Advisor: Professor Pierre Mothé Esteves
- *Science without Borders* scholar, academic exchange at **University of Lisbon (UL)**, Portugal

2008 – 2013

2012 – 2013

## AWARDS &amp; GRANTS

17. NSERC Banting Postdoctoral Fellowship  
(featured on: • Matter Group News) 2020 – 2021
16. MoISSI Workshop: Machine Learning and Chemistry: Challenges on the Way Forward  
@ University of Maryland, College Park, VA (*travel award*) 2019
15. CAS SciFinder Future Leaders Program  
(featured on: • C&EN News; • CAS Program for the 256<sup>th</sup> ACS National Meeting) 2018
14. ACS COMP Chemical Computing Group Excellence Award 2018
13. FSU's Graduate Student Research and Creativity Award 2018
12. ACS Graduate Research Symposium @ Indiana University, Bloomington, IN (*invited talk*) 2018
11. Machine Learning in Science and Engineering Symposium  
@ Carnegie Mellon University, Pittsburgh, PA (*travel award*) 2018
10. 67<sup>th</sup> Lindau Nobel Laureate Meeting (Chemistry), *invitation as young researcher*  
(featured on: • FSU News; • Brazilian Academy of Sciences; • the German newspaper *Süddeutsche Zeitung*) 2017
09. Philip Schlenoff Graduate Travel Award, grant used to attend the 67<sup>th</sup> Lindau Nobel Laureate Meeting 2017
08. IBM PhD Scholarship  
(featured on: • chem.fsu.edu/news; • FSU's Office of Graduate Fellowships and Awards) 2016
07. NSF XSEDE (TG-CHE160006): grant in the form of supercomputer time 2016 – 2018
06. Dr. Martin Luther King Jr. Book Stipend 2016
05. FSU's Congress of Graduate Students (COGS): grant to attend the 253<sup>rd</sup> ACS National Meeting 2016
04. Latin America-Caribbean (LAC) FSU Scholarship 2015 – 2018
03. Latin American Student Education and Research (LASER) Program Fellowship @ FSU 2014

02. Science without Borders Program and Scholarship @ UL 2012 – 2013
01. Gas Exploitation Oral Section winner: 6<sup>th</sup> Brazilian Meeting of R&D in Oil and Gas, as PRH01-ANP Scholar 2011

**PREPRINTS AND SUBMITTED ARTICLES** (s = authors contributed equally to this work.)

48. T. Gensch<sup>s</sup>, **G. P. Gomes**<sup>s</sup>, P. Friederich<sup>s</sup>, E. Peters, T. Gaudin, R. Pollice, K. Jorner, A. Nigam, M. L. D'Addario, M. S. Sigman, A. Aspuru-Guzik "A comprehensive platform for the discovery and understanding of organophosphorus ligands in catalysis", *preprint on ChemRxiv*: [link](#), **2021**, doi: 10.26434/chemrxiv.12996665 ► web app: <https://kraken.cs.toronto.edu>, [GitHub page](#); A collaboration with U of Utah, TU Berlin, KIT IBM Zurich, AstraZeneca
47. M. Christensen, L. Yunker, F. Adedeyi, F. Häse, L. Roch, T. Gensch, **G. P. Gomes**, T. Zepel, M. S. Sigman, A. Aspuru-Guzik, J. Hein "Data-science driven autonomous process optimization", *preprint on ChemRxiv*: [link](#), **2020** DOI: 10.26434/chemrxiv.13146404 ► A collaboration with Merck, UBC and U of Utah.
46. C. Lavigne, **G. P. Gomes**<sup>s</sup>, R. Pollice<sup>s</sup>, A. Aspuru-Guzik "Automatic discovery of chemical reactions using imposed activation", *preprint on ChemRxiv*, **2020**: [link](#), [GitHub page](#)

**PUBLICATIONS** (s = authors contributed equally to this work. ► Media and features highlighted with the publication.)

45. A. Nigam, R. Pollice, M. Krenn, **G. P. Gomes**, A. Aspuru-Guzik "Beyond Generative Models: Superfast Traversal, Optimization, Novelty, Exploration and Discovery (STONED) Algorithm for Molecules using SELFIES", *in print, Chem. Sci.*, **2021**, doi: 10.1039/D1SC00231G, *preprint on ChemRxiv*: [link](#), **2020**  
► Featured in Iwato Pen's cheminformatics blog: [link](#).
44. H. S. Auhim, B. L. Grigorenko, T. Harris, I. V. Polyakov, **G. P. Gomes**, I. V. Alabugin, P. J. Rizkallah, A. V. Nemukhin, D. D. Jones "Stalling chromophore maturation of the fluorescent protein Venus reveals the molecular basis of the final oxidation step", *in print, Chem. Sci.* **2021**, doi: 10.1039/D0SC06693A, *preprint on BioRxiv*: BIORXIV/2020/337386, **2020**
43. R. Pollice, P. Friederich, C. Lavigne, **G. P. Gomes**, A. Aspuru-Guzik "Organic Molecules with Inverted Gaps between First Excited Singlet and Triplet States and Appreciable Oscillator Strengths", *in print, Matter*, **2021**, *preprint on ChemRxiv*: [link](#), **2020**, DOI: 10.26434/chemrxiv.13087319 (*patent pending*)
42. **G. P. Gomes**, G. Xu, X. Zhu, L.-M. Chamoreau, O. Bistri-Aslanoff, S. Roland, I. V. Alabugin, M. Sollogoub "Mapping C-H...M interactions in confined spaces: ( $\alpha$ -ICyD<sup>Me</sup>)Au, Ag, Cu complexes reveal "contra-electrostatic H-bonds" masquerading as anagostic interactions", *in print, Chem. Eur. J.* **2021**, *preprint on ChemRxiv*: [link](#), **2020**, [GitHub page](#)
41. D. Diaz, S. D. Appavoo, A. F. Bogdanchikova, Y. Lebedev, T. J. McTiernan, **G. P. Gomes**, A. K. Yudin "Illuminating the dark conformational space of ring structures with dominant rotors", *Nature Chemistry* **2021**, *13*, 218, [GitHub page](#)  
► Selected as the cover for *Nature Chemistry*, Volume 13 Issue 3, March 2021: [link](#)
40. R. Pollice, **G. P. Gomes**, M. Aldeghi<sup>s</sup>, R. J. Hickman<sup>s</sup>, M. Krenn<sup>s</sup>, C. Lavigne<sup>s</sup>, M. L. D'Addario<sup>s</sup>, A. Nigam<sup>s</sup>, C.-T. Ser<sup>s</sup>, Z. Yao<sup>s</sup>, A. Aspuru-Guzik "Data-driven Strategies for Accelerated Materials Design", *Acc. Chem. Res.*, **2021**, *54*(4), 849 ► (• One of the most read papers *Accounts of Chemical Research* in February 2021)
39. **G. P. Gomes**<sup>s</sup>, R. Pollice<sup>s</sup>, A. Aspuru-Guzik "Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning", *Trends in Chemistry* **2021**, *3*(2), 96 special issue: "Machine Learning for Molecules and Materials" Guest editors: Rafael Gomez-Bombarelli (MIT) & Alexander Wiltschko (Google Brain), *preprint on ChemRxiv\_v1*: [link](#).  
► Selected as the cover for this special issue of *Trends in Chemistry*: [link](#)
38. S. Kaldas, C.-H. Tien, **G. P. Gomes**, S. Meyer, M. Sirvinskas, H. Foy, T. Dudding, A. K. Yudin "Oxidative Rearrangement of MIDA (*N*-Methyliminodiacetic Acid) Boronates: Mechanistic Insights and Synthetic Applications", *Org. Lett.* **2021**, *23*(2), 324, *preprint on ChemRxiv*: [link](#)
37. S. C. Davidson, **G. P. Gomes**, L. R. Kuhn, I. V. Alabugin, A. R. Kennedy, N. C. O. Tomkinson "Organocatalytic sulfoxidation", *Tetrahedron*, **2021**, *78*, 131784, ISSN 0040-4020
36. L. R. Mills, J. J. Monteith, **G. P. Gomes**, A. Aspuru-Guzik, S. A. L. Rousseaux "The cyclopropane ring as a reporter of radical leaving-group reactivity for Ni-catalyzed C(sp<sup>3</sup>)-O arylation", *J. Am. Chem. Soc.* **2020**, *142* (30), 13246, *preprint on ChemRxiv*: [link](#) ► (Featured on *OPR&D* as interesting reaction to process R&D chemists: Zhao et al., *Org. Process Res. Dev.* **2020**, acs.oprd.0c00419.)

35. P. Friederich, **G. P. Gomes**, R. D. Bin, A. Aspuru-Guzik, D. Balcells “Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska’s Complex”, *Chem. Sci.* **2020**, *11*, 4584, *preprint on ChemRxiv: [link](#), GitHub page: [Vaska’s space](#)*  
▶ (• Selected as the inside front cover for *Chemical Science: [link](#)*; • Featured on the Matter Group [website](#))
34. E. Gonzalez-Rodriguez, M. Abdo, **G. P. Gomes**, S. Ayad, N. P. Tsvetkov, F. D. White, K. Hanson, I. V. Alabugin “Twofold  $\pi$ -Extension of Polyarenes via Double and Triple Radical Alkyne peri-Annulations: Radical Cascades Converging on the Same Aromatic Core”, *J. Am. Chem. Soc.* **2020**, *142* (18), 8352, *preprint on ChemRxiv: [link](#)*  
▶ (Highlighted on: • *Synfacts* **2020**, *16*, 794 “Peri-Peri: Spicy Radical Double Annulations”)
33. Q. Elliott, **G. P. Gomes**, C. J. Evoniuk, I. V. Alabugin “Testing the Limits of Radical-Anionic CH-Amination: a 10-Million-Fold Decrease in Basicity Opens a New Path to Hydroxyisoindolines via a Mixed C-N/C-O-Forming Cascade”, *Chem. Sci.* **2020**, *5*, 369, *preprint on ChemRxiv: [link](#)*
32. R. Lee, E. Cagle, B. Bashrum, E. Walters, J. Massey, M. Zanghi, C. Birchfield, D. French, J. Joy, **G. P. Gomes**, P. A. Wiget, “Electronic donation or steric contraction: a spectroscopic and structural analysis of medium-sized constrained rings for potential long-range hyperconjugation”, *J. Org. Chem.*, **2019**, *84*(16), 9897
31. **G. P. Gomes**, A. Wimmer, J. M. Smith, B. Koenig, I. V. Alabugin “CO<sub>2</sub> or SO<sub>2</sub>: Should it stay, or should it go?”, *J. Org. Chem.*, **2019**, *84* (10), 6232, *preprint on ChemRxiv*
30. A. Hughes, **G. P. Gomes**, I. V. Alabugin, “Stereolectronic Influence of a “Spectator” Propargylic Substituent Can Override Aromaticity Effects in Radical *Peri*-cyclizations on Route to Expanded Polyaromatics”, *J. Org. Chem.*, **2019**, *84* (4), 1853
29. **G. P. Gomes**, A. E. Morrison, G. B. Dudley, I. V. Alabugin “Optimizing amine-mediated alkyne-allene isomerization to improve benzannulation cascades: synergy between theory and experiments”, *Eur. J. Org. Chem.*, **2019**, 512, *Special Issue: Catalyst Design*
28. V. A. Vil’, **G. P. Gomes**, M. V. Ekimova, K. A. Lyssenko, G. I. Nikishin, I. V. Alabugin, A. O. Terent’ev “Five roads that converge at the cyclic peroxy-Criegee intermediates: BF<sub>3</sub>-catalyzed synthesis of  $\beta$ -hydroperoxy- $\beta$ -peroxylactones”, *J. Org. Chem.* **2018**, *83* (21), 13427
27. **G. P. Gomes**, Y. Loginova, S. Z. Vatsadze, I. V. Alabugin “Isocyanides as Stereoelectronic Chameleons: The Donor-Acceptor Dichotomy in Radical Additions”, *J. Am. Chem. Soc.*, **2018**, *140* (43), 14272, *preprint on ChemRxiv: [link](#)*  
▶ (Highlighted on: • *ACS Axial*; • *Colorblind Chemist*)
26. I. V. Alabugin, **G. P. Gomes**, M. Abdo, “Hyperconjugation”, *WIREs Comput Mol Sci.*, **2018**;e1389  
▶ (• *Top 10% 2018-2019 downloaded papers from WIREs Comput Mol Sci.*)
25. **G. P. Gomes** & I. V. Alabugin “Stereoelectronic Effects: Analysis by Computational and Theoretical Methods”, chapter 15 for the book “*Applied Theoretical Organic Chemistry*”, pp. 451-502, **2018**, Ed: Dean Tantillo
24. Y. A. Yaremenko<sup>§</sup>, **G. P. Gomes**<sup>§</sup>, P. S. Radulov, R. A. Novikov, V. V. Chernyshev, A. A. Korlyukov, G. I. Nikishin, I. V. Alabugin, A. O. Terent’ev “Ozone-free synthesis of ozonides: Assembling bicyclic structures from 1,5-diketones and hydrogen peroxide” *J. Org. Chem.*, **2018**, *83* (8), 4402
23. N. P. Tsvetkov, E. Gonzalez-Rodriguez, A. Hughes, **G. P. Gomes**, F. D. White, I. V. Alabugin “Radical Alkyne Peri-annulations for Synthesis of Functionalized Phenalenes, Benzanthenes, and Olympicene”, *Angew. Chem. Int. Ed.*, **2018**, *57*, 3651 ▶ (• *Top 5% of ACIE’s output*. Featured on: • *Synfacts* **2018**, *14* (05), 473 “*peri*-Annulation for Polyaromatic Hydrocarbons”; • *FSU News*, reproduced on: • *phys.org*; • *nsf.gov/news*; • *sciencedaily.com*; • *EurekAlert!*)
22. V. A. Vil’, **G. P. Gomes**, O. V. Bityukov, M. A. Syroeshkin, K. A. Lyssenko, G. I. Nikishin, I. V. Alabugin, A. O. Terent’ev “Interrupted Baeyer-Villiger Rearrangement: Building A Stereoelectronic Trap for the Criegee Intermediate”, *Angew. Chem. Int. Ed.*, **2018**, *57*, 3372 ▶ (• *Top 5% of ACIE’s output*. Featured on: • *Chemical & Engineering News*)
21. K. N. Sedenkova, E. B. Averina, Y. K. Grishin, J. V. Kolodyazhnaya, V. B. Rybakov, T. S. Kuznetsova, A. Hughes, **G. P. Gomes**, I. V. Alabugin, N. S. Zefirov “Substituent effects on stereoselectivity of dihalocarbene reactions with cyclohexadiene and on the reactivity of bis-dihalocyclopropanes in electrophilic nitrations on route to pyrimidine *N*-oxides” *Org. Biom. Chem.*, **2017**, *15*, 9433

20. C. J. Evoniuk, **G. P. Gomes**, S. Hill, F. Satoshi, I. V. Alabugin “Coupling C-H activation, N-H deprotonation and Oxidation: metal-free C(sp<sup>3</sup>)-H aminations with unprotected anilines” *J. Am. Chem. Soc.*, **2017**, *139* (45), 16210  
▶ (featured on: • *Synfacts* **2018**, *14* (02), 144 “Expanded N-Heterocycles through C(sp<sup>3</sup>)-H Amination”; • in the top 20 most-read *JACS* papers in Oct-Nov 2017)
19. T. Harris, **G. P. Gomes**, R. Clark, S. Ayad, V. V. Lobodin, K. Hanson, I. V. Alabugin “Twisted chiral cyclodecynes and remote activation of click reactivity” *Chem*, **2017**, *3* (4), 629 ▶ (• *video-summary of the paper*; • *FSU News*)
18. N. H. Park, **G. P. Gomes**, M. Fevre, G. O. Jones, I. V. Alabugin, J. L. Hedrick, “Organocatalyzed Synthesis of Fluorinated Poly(aryl thioethers)” *Nature Communications*, **2017**, *8*, 166; ▶ (a collaboration with *IBM Research, San Jose, CA*. Featured on: • *Plastic News*; • *Synfacts* **2017**, *13* (10), 1035 “Salt-Free Polymerization Yields Fluorinated Poly(aryl thioether)s”)
17. E. Juaristi, **G. P. Gomes**, A. O. Terent’ev, R. Notario, I. V. Alabugin “Stereolectronic Interactions as a Probe for the Existence of the Intramolecular  $\alpha$ -Effect”, *J. Am. Chem. Soc.*, **2017**, *139* (31), 10799
16. P. Poonptana, **G. P. Gomes**, T. Hurrle, K. Chardon, S. Bräse, K-S. Masters, I. V. Alabugin “Formaldehyde-Extruding Homolytic Aromatic Substitution via C→O Transposition: Evolution of a Contaminating Side-Reaction to ‘Traceless-Linker’ access to Congested Biaryl Bonds” *Chem. Eur. J.*, **2017**, *23*, 9091 ▶ (featured: • *Hot Paper* in *Chem. Eur. J.*)
15. **G. P. Gomes**<sup>§</sup>, C. J. Evoniuk<sup>§</sup>, M. Ly, I. V. Alabugin “Changing the path of least resistance, or access to *endo*-dig products *via* a sequence of three *exo*-trig transition states: electronic effects in homoallylic ring expansion cascades of alkenyl isonitriles” *Org. Biom. Chem.*, **2017**, *15*, 4135
14. C. J. Evoniuk<sup>§</sup>, **G. P. Gomes**<sup>§</sup>, M. Ly, F. D. White, I. V. Alabugin “Coupling radical homoallylic expansions with C-C fragmentations for the synthesis of heteroaromatics: Quinolines from reactions of *o*-alkenylarylisonitriles with aryl, alkyl and perfluoroalkyl radicals” *J. Org. Chem.*, **2017**, *82* (8), 4265 ▶ (featured on: • *Synfacts* **2017**, *13* (06), 582 “Synthesis of Quinolines From *o*-Alkenylaryl Isonitriles”; • *organic-chemistry.org*)
13. **G. P. Gomes**<sup>§</sup>, Y. A. Yaremenko<sup>§</sup>, P. S. Radulov, R. A. Novikov, V. V. Chernyshev, A. A. Korlyukov, G. I. Nikishin, A. O. Terent’ev, I. V. Alabugin “Stereolectronic Control in the Ozone-Free Synthesis of Ozonides” *Angew. Chem. Int. Ed.*, **2017**, *56*, 4955
12. **G. P. Gomes** & I. V. Alabugin “Drawing Catalytic Power from Charge Separation: Stereolectronic and Zwitterionic Assistance in the Au(I)-Catalyzed Bergman Cyclization” *J. Am. Chem. Soc.*, **2017**, *139* (9), 3406
11. S. Umedu, **G. P. Gomes**, M. Sakae, T. Yoshinaga, K. Matsumoto, T. Iwata, I. Alabugin, M. Shindo “Regioselective One-pot Synthesis of Triptycenes via Triple-Cycloadditions of Arynes to Ynolates” *Angew. Chem. Int. Ed.*, **2016**, *56*, 1298 ▶ (featured on: • *Synfacts* **2017**, *13* (03), 253 “Three Benzynes and the Ynolate”)
10. S. Z. Vatsadze, Y. Loginova, **G. P. Gomes**, I. V. Alabugin “Stereolectronic Chameleons: The Reversal of Donor-Acceptor Properties of Common Functional Groups by a Geometric Change” *Chem. Eur. J.*, **2016**, *23*, 3225 ▶ (Web of Science’s top 1% Chemistry highly cited papers for Nov/Dec 2017; *Frontspiece of Chemistry – A European Journal*)
09. K. Pati, **G. P. Gomes**, I. V. Alabugin “Combining Traceless Directing Groups with Hybridization Control of Radical Reactivity: from Skipped Enynes to Defect-Free Hexagonal Frameworks” *Angew. Chem. Int. Ed.*, **2016**, *55*, 11633
08. T. Harris, **G. P. Gomes**, R. Clark, I. V. Alabugin, “Domino Fragmentations in Traceless Directing Groups of Radical Cascades: Evidence for the Formation of Alkoxy Radicals via C-O Scission” *J. Org. Chem.*, **2016**, *81* (14), 6007  
▶ (featured on: • *sciencing.net*)
07. E. Berry<sup>§</sup>, **G. P. Gomes**<sup>§</sup>, A. MacLean, J. R. Martin, P. A. Wiget, “Discovery of a new type of Perlin effect in a conformationally constrained oxocane” *J. Org. Chem.*, **2016**, *81* (13), 5740
06. K. Pati, **G. P. Gomes**, T. Harris, I. V. Alabugin “Fused Catechol Ethers from Gold (I)-Catalyzed Intramolecular Reaction of Propargyl Ethers with Acetals” *Org. Lett.*, **2016**, *18* (5), 928
05. **G. P. Gomes**, V. A. Vil’, A. Terent’ev and I. V. Alabugin, “Stereolectronic Source of the Anomalous Stability of Bis-peroxides” *Chem. Sci.*, **2015**, *6*, 6783 ▶ (featured on: • *Chemistry World*; • NBO’s features website; • chem.fsu.edu/News. Behind the scenes on: • medium.com)
04. K. Pati, C. Michas, D. Allenger, I. Piskun, P. S. Coutros, **G. P. Gomes**, I. V. Alabugin, “Synthesis of Functionalized Phenanthrenes via Regioselective Oxidative Radical Cyclization” *J. Org. Chem.*, **2015**, *80* (23), 11706
03. E. Stoyanov & **G. P. Gomes** “*Tert*-Butyl Carbocation in Condensed Phases: Stabilization via Hyperconjugation, Polarization and Hydrogen Bonding” *J. Phys. Chem. A*, **2015**, *119*, 8619

02. K. Pati, **G. P. Gomes**, T. Harris, A. Hughes, H. Phan, T. Banerjee, K. Hanson, I. V. Alabugin “Traceless Directing Groups in Radical Cascades: From Oligoalkynes to Fused Helicenes without Tethered Initiators” *J. Am. Chem. Soc.*, **2015**, *137*, 1165
01. I. V. Alabugin, S. Bresch, **G. P. Gomes** “Orbital Hybridization: A Key Electronic Factor in Control of Structure And Reactivity” *J. Phys. Org. Chem.*, **2014**, *28*, 147 ► (one of the *most accessed* papers on: • *JPOC* between 10/2015-09/2016 & 02/2016-08/2017 • department’s most read paper on *ResearchGate* in October–November 2017; featured on: • *amphoteros.com*)

## HONORS & MEDIA

- |   |      |
|---|------|
| 1. Selected for the Univeristy of Michigan Ann Arbor “ <i>NextProf:Science</i> ” workshop   | 2021 |
| 2. Selected for the 2021 Univeristy of Chicago Future Faculty Conference  | 2021 |
| 3. Featured on the “ <i>Next Great Impossible</i> ” series by Merck/Milipore-Sigma ( <a href="#">link</a> )   | 2020 |
| 4. <i>LatinXChem</i> featured on C&En News ( <a href="#">link</a> )   | 2020 |
| 5. One of the winner teams with “Robo-boat for oil spill management” on <i>PuebloScience</i> ’s Hackathon for Science Education @ UofT, Toronto, ON | 2019 |
| 6. Featured on Florida State University’s College of Arts & Sciences’ Spectrum Magazine with the article “ <i>Scientific Sensation</i> ”            | 2019 |
| 7. Selected for IUPAC’s Periodic Table of Younger Chemists as “Yttrium”   | 2018 |
| 8. Featured as a Florida State University Student Star  | 2018 |
| 9. Florida State University Fellows Society ( <i>inducted</i> )   | 2017 |
| 10. FSU Student Employee of the Year Award ( <i>nomination</i> )  | 2017 |
| 11. Honorable Mention: XXXII <i>Jornada Giulio Massarani de Iniciação Científica</i> , as a CNPq Scholar  | 2010 |

## MENTORED RESEARCH & WORK EXPERIENCE

- |   |             |
|---|-------------|
| <ul style="list-style-type: none"> <li>▪ Postdoctoral Researcher at UofT, Aspuru-Guzik Group           <ul style="list-style-type: none"> <li>• AI for Catalysis, Reaction Discovery, and Optimization. Autonomous Labs.</li> <li>• Development of platforms for the inverse-design of catalysts and energy materials.</li> </ul> </li> </ul> | 2019 – 2021 |
| <ul style="list-style-type: none"> <li>▪ Research Assistant (RA) at FSU, Alabugin Group           <ul style="list-style-type: none"> <li>• Computational and Physical Organic Chemistry.</li> <li>• Extensive work on the study and control of chemical reactions with stereoelectronic effects.</li> </ul> </li> </ul>                       | 2014 – 2018 |
| <ul style="list-style-type: none"> <li>▪ Internship at (Center for Structural Chemistry) CQE-FCUL, Advisor: Dr. Maria José Lourenço           <ul style="list-style-type: none"> <li>• “Development of electrodes with reduced graphene oxide”</li> </ul> </li> </ul>   | 2012 – 2013 |
| <ul style="list-style-type: none"> <li>▪ Undergraduate researcher at INTERLAB-IQ/UFRJ, Advisor: Prof. Pierre Mothé Esteves           <ul style="list-style-type: none"> <li>• PRH01-ANP scholar, undergrad thesis: “Development and Molecular Study of Methane Hydrates Inhibitors”</li> </ul> </li> </ul>                                    | 2010 – 2012 |
| <ul style="list-style-type: none"> <li>• CNPq scholar, computational chemist: “Theoretical Study of Electrophilic Aromatic Nitration”</li> </ul>  | 2008 – 2010 |
| <ul style="list-style-type: none"> <li>▪ CERN’s GISELA-GRID at IF/UFRJ           <ul style="list-style-type: none"> <li>• High performance computing (HPC) manager and infrastructure administrator</li> </ul> </li> </ul>  | 2012        |

## MENTORING EXPERIENCE

- Mentor to Graduate Students:
  - Cher-Tian Ser (UofT, 2020 – 2021): “Inverse-designing Suzuki-coupling catalysts with machine-learning”
  - Riley Hickman (UofT, 2019 – 2021): “Bayesian methods for the inverse-design of catalysts”
  - Michael Lindner D’Addario (UofT, 2020 – 2021): “Designing pipelines for inverse-design of catalysts with machine-learning”
  - Aleksandra Holownia (UofT, 2019 – 2020): “Computational strategies for the development of a MIDA-protected boryl-radical generation”
  - Sherif Kaldas (UofT, 2019 – 2020): “Computational studies of Pd-catalyzed allylic rearrangements”
  - Edgar Gonzalez-Rodriguez (FSU, 2018): “Mechanistic studies of radical cascade cyclizations”

- Mentor to Undergraduate Students:
  - Benjamin Ding (UofT, 2020 – 2021): “Finding new OLED materials with high-throughput screening” co-mentored with Dr. Robert Pollice
  - Lucinda Zhu (UofT, 2020 – 2021): “Developing computational frameworks for discovering new organocatalysts”
  - Akshatkumar Nigam (UofT, 2019 – 2021): “Applying genetic algorithms for the development and discovery of new catalysts”
  - Shelby Davis (FSU, Honors Thesis, 2018):  
“Weaving Together Alkynes to Form Fully Six-Membered Polyaromatic Frameworks”
  - Nicholas Bigerton (FSU, Directed Individual Study, 2014 – 2015):  
“Computational Studies of Triple-Cycloadditions of Alkynes to Ynolates”

## LEARNING & TEACHING EXPERIENCE

- Neural Networks Programming Course (DAT112) @ SciNet/UofT, Toronto, ON, Canada (Spring 2019)
- Graduate school coursework: Physical Organic Chemistry, Density Functional Theory, Advanced Organic Synthesis, Advanced Materials Chemistry, Advanced Polymer Chemistry, Group Theory & Inorganic Chemistry
- Teaching Assistant (TA) at FSU (2015 – 2017): Organic Chemistry II: Laboratory & Recitation.
- Teaching Assistant at *descomplica.com.br*, 3<sup>rd</sup> most innovative company of Latin America by *Fast Company* (2010–2014)
- Teaching Assistant at the Institute of Chemistry, UFRJ (2010): Experimental Organic Chemistry I and II

## INVITED SEMINARS & PRESENTATIONS

1. "Building a Universal Data Science Workflow for Monodentate Organophosphorus Ligands" *invited seminar*, 2021 AIChE Annual Meeting in Boston, MA, Topical Conference (Applications of Data Science to Molecules and Materials): "*Applications of Data Science in Catalysis and Reaction Engineering*" (2021)
2. "Designing Catalysts with an Augmented Genetic Algorithm" *invited seminar*, ACS Meeting Fall, special symposium (CATL division): "*Accelerating Catalysis Research with Machine Learning*" (2021) – *to be delivered virtually*
3. "Building a Universal Data Science Workflow for Monodentate Organophosphorus Ligands" @ JAWS (2021) – *to be delivered virtually*
4. "Building a Universal Data Science Workflow for Monodentate Organophosphorus Ligands" *invited seminar* @ Post-Grad Program in Chemistry, UFRJ, RJ, Brazil (2021) – *to be delivered virtually*
5. Mapping the Property Space of Monodentate Organophosphorus Ligands for Catalysis" *invited seminar* @ Fordham University, New York City, NY (2021) – *delivered virtually*
6. "Navigating through the Maze of Homogeneous Catalyst Design with Machine Learning" *invited seminar* @ Latin-American Network for Theoretical Physical Chemistry – *Red Latinoamericana de Fisicoquímica Teórica* (2021) – *delivered virtually*, [YouTube link](#)
7. "Mapping the Property Space of Monodentate Organophosphorus Ligands for Catalysis" *invited seminar*, ACS Meeting Spring, special symposium (CINF division): "*Machine Learning and AI for Organic Chemistry*" (2021) – *delivered virtually*
8. "Mapping the Property Space of Monodentate Organophosphorus Ligands for Catalysis", Aspuru-Guzik Group Meeting @ University of Toronto, Toronto, ON (2021) – *delivered virtually*
9. "Computational strategies for learning how to control chemical reactivity" *invited seminar* @ Carnegie Mellon University Chemical Engineering, Pittsburgh, PA (2021) – *delivered virtually*
10. "Computational strategies for learning how to control chemical reactivity" *invited seminar* @ Carnegie Mellon University Chemistry, Pittsburgh, PA (2021) – *delivered virtually*
11. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Heidelberg Institute for Theoretical Studies, Germany (2020) – *delivered virtually*
12. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Physical, Theoretical and Computational Chemistry (PTC) seminar series for the Chemical Institute of Canada (2020) – *delivered virtually*

13. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Wu Group Meeting @ University of Houston, Houston, TX (2020) – *delivered virtually*
14. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Department Seminar @ UFSCar, SP, Brazil (2020) – *delivered virtually*
15. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Tormena Group Meeting @ UNICAMP, SP, Brazil (2020) – *delivered virtually*
16. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Duarte Group Meeting @ Oxford University, UK (2020) – *delivered virtually*
17. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Esteves Group Meeting @ Institute of Chemistry, Federal University of Rio de Janeiro, RJ, Brazil (2020) – *delivered virtually*
18. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Chemical Physics (Segal group) Group Meeting @ University of Toronto, Toronto, ON (2020) – *delivered virtually*
19. "Computational strategies for learning how to control chemical reactivity", *invited seminar* @ Rice University, Houston, TX (2020) – *canceled due to COVID-19 travel restrictions*
20. "Computational strategies for learning how to control chemical reactivity", *invited seminar* @ University of Houston, Houston, TX (2020) – *canceled due to COVID-19 travel restrictions*
21. "Computational strategies for learning how to control chemical reactivity", *invited seminar* @ Southern Methodist University, Dallas, TX (2019)
22. "Accurate and Explainable Machine Learning of Chemical Reactivity in Transition Metal Complexes", [Pascal Friederich](#), G. P. Gomes, R. De Bin, D. Balcells, A. Aspuru-Guzik @ 2019 MRS Fall Meeting, Boston, MA (2019)
23. "Machine Learning Reactivity in the Chemical Space of Vaska's Complex", 47<sup>th</sup> Physical Organic Minisymposium (POMS) @ York University, Toronto, ON (2019)
24. "Computational strategies for learning how to control chemical reactivity", *invited seminar* @ Iowa State University, Ames, IA (2019)
25. "Computational strategies for learning how to control chemical reactivity", *invited seminar* @ CINVESTAV, Mexico City, Mexico (2019)
26. "Computational strategies for learning how to control chemical reactivity", *invited seminar* @ UNAM, Mexico City, Mexico (2019)
27. "Drawing Catalytic Power from Charge Separation: Stereoelectronic and Zwitterionic Assistance in the Au(I)-Catalyzed Bergman Cyclization", ACS COMP Awards poster presentation @ 256<sup>th</sup> ACS Meeting, Boston, MA (2018)
28. "Taming Oxygen-Rich Systems with Stereoelectronic Effects", oral presentation @ 256<sup>th</sup> ACS Meeting, Boston, MA (2018)
29. "Drawing Catalytic Power from Charge Separation: Stereoelectronic and Zwitterionic Assistance in the Au(I)-Catalyzed Bergman Cyclization", poster presentation @ CAS, Columbus, OH (2018)
30. "Taming Oxygen-Rich Systems with Stereoelectronic Effects", oral presentation @ Graduate Research Symposium, Indiana University, Bloomington, IN (2018)
31. "Taming Oxygen-Rich Systems with Stereoelectronic Effects", *invited seminar* @ Institute of Chemistry, Federal University of Rio de Janeiro, RJ, Brazil (2018)
32. "Taming Oxygen-Rich Systems with Stereoelectronic Effects", *invited seminar* @ Doyle Group, Princeton University, Princeton, NJ (2018)
33. "Taming Oxygen-Rich Systems with Stereoelectronic Effects", *invited seminar* @ Aspuru-Guzik Group, Harvard University, Cambridge, MA (2018)
34. "Taming Peroxides with Stereoelectronic Effects: Stereoelectronic Control in the Ozone-Free Synthesis of Ozonides", oral presentation, 4<sup>th</sup> year-talk @ FSU Organic Seminar, Tallahassee, FL (2018)
35. "Taming Peroxides with Stereoelectronic Effects: Stereoelectronic Control in the Ozone-Free Synthesis of Ozonides", poster presentation @ FloHet 2018, Gainesville, FL (2018)
36. "Reinventing cycloaromatization reactions: the diradical/zwitterion dichotomy", [I. V. Alabugin](#), G. P. Gomes @ WATOC 2017, Munich, Germany (2017)
37. "Supramolecular Effects in Radical Chemistry", poster presentation @ 253<sup>rd</sup> ACS Meeting, San Francisco, CA (2017)

38. “Employing stereoelectronic effects to design organocatalyzed S→F exchange towards functional polythioethers”, *invited seminar @ IBM Research Center, Almaden, CA (2016)*
39. “Designing Cascade Cyclizations and Fragmentations with Stereoelectronic Effects: Controlling Radical Arrival and Departure”, *invited seminar @ Todd Martinez Group, Stanford University, CA (2016)*
40. “Stereoelectronic effects are in control of reactivity”, poster presentation @ SETCA (2016)
41. “Stereoelectronic effects are in control of reactivity”, oral presentation, 2<sup>nd</sup> year-talk @ FSU Organic Seminar, Tallahassee, FL (2016)
42. “Stereoelectronic effects are in control of reactivity”, oral presentation @ 92<sup>nd</sup> FAME, (2016)
43. “Stereoelectronic effects are in control: from the anomalous stability of bis-peroxides to radical cascade cyclizations”, poster presentation @ 251<sup>th</sup> ACS Meeting, San Diego, CA (2016)
44. Computational Design of New Routes to Graphene Nanoribbons, poster presentation @ FSU Digitech (2015)
45. “Theoretical Study of Electrophilic Aromatic Nitration”, poster presentation @ XV SBQt (2009)
46. XXXI, XXXII and XXXIV Jornada Giulio Massarani de Iniciação Científica, oral presentations (2009 – 2013)

#### WORKSHOPS, SYMPOSIUMS & CONFERENCES

47. University of Chicago Future Faculty Conference, Chicago, IL – *virtual* (2021)
48. NextProf:Science Workshop at University of Michigan Ann Arbor, MI – *virtual* (2021)
49. Workshop: “*Materials Acceleration Platforms: AI, Robotics and Computation for Accelerated Discovery*” @ University of Toronto, Toronto, ON (2020)
50. MolSSI Workshop: Machine Learning and Chemistry: Challenges on the Way Forward @ University of Maryland, College Park, VA (2019)
51. International Meeting on Artificial Intelligence and its Applications (RIIAA @ MEX 2.0), Mexico City, Mexico (2019)
52. DARPA Accelerated Materials Discovery Kick-Off Meeting, Arlington, VA (2019)
53. CAS SciFinder Future Leaders Program @ Columbus, OH (2018)
54. Machine Learning in Science and Engineering Symposium @ Carnegie Mellon University, Pittsburgh, PA (2018)
55. MLx18: A Machine Learning Conference at Florida State University, FSU, Tallahassee, FL (2018)
56. 67<sup>th</sup> Lindau Nobel Laureate Meeting (Chemistry), Lindau, Germany (2017)
57. Q-Chem 5.0 User Workshop, San Francisco, CA (2017)
58. 24<sup>th</sup> Winter Inter-American Photochemical Society Conference (2015)
59. School of Advanced Characterization of Nanomaterials of INMETRO (2014)
60. pDynamo Workshop & Molecular Simulation (2013) at University of Sao Paulo, SP – Brazil
61. School of Advanced Studies in Applied Thermodynamics: Monte Carlo Simulations (2011)

#### SERVICE & SCHOLARLY REVIEWS

- Early Career Board member of *Journal of Chemical Information and Modeling* (2021 – 2023, [link](#))
- Organizing Committee (& co-organizer for the catalysis mini-symposium #LatinXChemCat) for *LatinXChem*, a virtual forum for the worldwide Latin-American chemistry community, with over 1200 posters in its 1<sup>st</sup> edition ([link](#)) ► featured on: • *C&EN News*; • *UNICAMP News*
- Reviewer for the 1<sup>st</sup> Global Inorganic Discussion Weekday Virtual Poster Competition (#gidw2020, [link](#))
- Ongoing peer reviewer for: *Chemistry of Materials*, *ACS Catalysis*, *Journal of Chemoinformatics*, *Journal of Chemical Information and Modeling*, *Nature Computational Science*, *Nature Communications*, *Accounts of Chemical Research*, *Chemical Science*, *ChemistrySelect*, *ACS Omega*
- Opinions on RSC’s *Chemistry World* article “Language-based software’s accurate predictions translate to benefits for chemists” as a machine learning & organic chemistry researcher (2019)
- *PuebloScience*’s Hackathon for Science Education @ UofT, Toronto, ON (2019)
- FSU’s Dr. Martin Luther King Jr. Book Stipend Selection Committee, *invited* (2017)
- Graduate Student Commission for Invited Lectures at FSU Dept. of Chemistry and Biochemistry (2016 – 2017)
- Member of Students Commission of Chemistry Institute at UFRJ (2009 – 2012)
- Organization Commission of the XVII, XIX and XX Weeks of Chemistry of UFRJ (2009 – 2012)



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## PROGRAMMING, SKILLS & SOFTWARES

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- Phosphines database web application & development ([link](#))
- Machine learning packages: Keras, TensorFlow, PyTorch, GPy, scikit-learn
- Programming languages: Python, Bash, MATLAB, Mathematica
- Quantum chemistry packages: Gaussian, xtb, crest, Q-Chem, ORCA, Jprogdyn, TeraChem, Psi4
- Molecular analysis: NBO, (N)EDA, NICS-XY, SAPT, ACID, FOD, Aroma
- Data visualization: Matplotlib, Seaborn, Prism
- Molecular visualization: GaussView, ChemCraft, CYLView, UCSF Chimera, PyMol, JMol

†: most of the information is hyperlinked in the pdf version of this CV

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