

EDUCATION & TRAINING

University of Toronto (UofT), Department of Chemistry and Department of Computer Science Toronto, ON, Canada

- NSERC Banting Postdoctoral Fellow
 - Project titled: “*Designing Catalysts with Artificial Intelligence*” April 2020 – present
- Postdoctoral Research Fellow, Advisor: Professor Alán Aspuru-Guzik 2019 – present
 - Visiting scholar at **Vector Institute for Artificial Intelligence** 2019 – present
 - Developed platforms for inverse-designing catalysts with artificial intelligence
 - Provided key structural and mechanistic insights to various challenges in organic chemistry with computational methods

Florida State University (FSU), Department of Chemistry and Biochemistry Tallahassee, FL, USA

- Ph.D. in Chemistry, GPA 4.0, Advisor: Professor Igor V. Alabugin 2014 – 2018
 - *in-flight* M.Sc. in Chemistry 2014 – 2016
 - Ph.D. Dissertation entitled: “*Controlling Chemical Reactivity with Stereoelectronic Effects*”

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 2008 – 2013
 - *Science without Borders* scholar, academic exchange at **University of Lisbon (UL)**, Portugal 2012 – 2013

AWARDS & GRANTS

1. NSERC Banting Postdoctoral Fellowship 2020 – present
(featured on: • Matter Group News)
2. Co-writer for grant (HR00111920097) “*Accelerated Materials Discovery*” 2019 – present
from Defense Advanced Research Projects Agency (DARPA). A collaboration between UofT, UIUC, UBC, UGlasgow, and Allchemy. Project: Molecular Accelerated Discovery of Novelty Enabled by Synthetic Systems (MADNESS)
3. MolSSI Workshop: Machine Learning and Chemistry: Challenges on the Way Forward 2019
@ University of Maryland, College Park, VA (*travel award*)
4. CAS SciFinder Future Leaders Program 2018
(featured on: • C&EN News; • CAS Program for the 256th ACS National Meeting)
5. ACS COMP Chemical Computing Group Excellence Award 2018
6. FSU’s Graduate Student Research and Creativity Award 2018
7. ACS Graduate Research Symposium @ Indiana University, Bloomington, IN (*invited talk*) 2018
8. Machine Learning in Science and Engineering Symposium 2018
@ Carnegie Mellon University, Pittsburgh, PA (*travel award*)
9. 67th Lindau Nobel Laureate Meeting (Chemistry), *invitation as young researcher* 2017
(featured on: • FSU News; • Brazilian Academy of Sciences; • the German newspaper *Süddeutsche Zeitung*)
10. Philip Schlenoff Graduate Travel Award: grant used to attend the 67th Lindau Nobel Laureate Meeting 2017
11. IBM PhD Scholarship 2016
(featured on: • chem.fsu.edu/news; • FSU’s Office of Graduate Fellowships and Awards)
12. NSF XSEDE (TG-CHE160006): grant in the form of supercomputer time 2016 – 2018
13. Dr. Martin Luther King Jr. Book Stipend 2016
14. FSU’s Congress of Graduate Students (COGS): grant to attend the 253rd ACS National Meeting 2016
15. Latin America-Caribbean (LAC) FSU Scholarship 2015 – 2018
16. Latin American Student Education and Research (LASER) Program Fellowship @ FSU 2014
17. Science without Borders Program and Scholarship @ UL 2012 – 2013
18. Gas Exploitation Oral Section winner: 6th Brazilian Meeting of R&D in Oil and Gas, as PRH01-ANP Scholar 2011

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

47. M. Christensen, L. Yunker, F. Adedeji, 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**§, R. Pollice§, A. Aspuru-Guzik “Automatic discovery of chemical reactions using imposed activation”, *preprint on ChemRxiv*, **2020**: [link](#), [GitHub page](#)
45. 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”, *preprint on BioRxiv*: BIORXIV/2020/337386, **2020**
44. 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”, *preprint on ChemRxiv*: [link](#), **2020** ► Featured in Iwatobi Pen’s cheminformatics blog: [link](#).
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”, *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: (α -ICyD^{Me})Au, Ag, Cu complexes reveal “contra-electrostatic H-bonds” masquerading as anagostic interactions”, *preprint on ChemRxiv*: [link](#), **2020**, [GitHub page](#)

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

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§, R. J. Hickman§, M. Krenn§, C. Lavigne§, M. L. D’Addario§, A. Nigam§, C.-T. Ser§, Z. Yao§, A. Aspuru-Guzik “Data-driven Strategies for Accelerated Materials Design”, *Acc. Chem. Res.*, **2021**, *54*(4), 849
39. **G. P. Gomes**§, R. Pollice§, 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*³)–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 π -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 "CO₂ or SO₂: 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, "Stereo-electronic 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: BF₃-catalyzed synthesis of β -hydroperoxy- β -peroxylactones", *J. Org. Chem.* **2018**, 83 (21), 13427
27. **G. P. Gomes**, Y. Loginova, S. Z. Vatsadze, I. V. Alabugin "Isocyanides as Stereo-electronic 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 "Stereo-electronic 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[§], **G. P. Gomes**[§], 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 Stereo-electronic 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(sp³)-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(sp³)-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 cyclodecyne and remote activation of click reactivity" *Chem*, **2017**, 3 (4), 629 ▶ (• *video-summary of the paper*. Featured on: • *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 "Stereo-electronic Interactions as a Probe for the Existence of the Intramolecular α -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 \rightarrow O Transposition: Evolution of a Contaminating Side-Reaction to 'Traceless-Linker' access to Congested Biaryl Bonds" *Chem. Eur. J.*, **2017**, 23, 9091 ▶ (featured as: • *Hot Paper* in *Chem. Eur. J.*)
15. **G. P. Gomes**[§], C. J. Evoniuk[§], 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[§], **G. P. Gomes[§]**, 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[§]**, Y. A. Yaremenko[§], P. S. Radulov, R. A. Novikov, V. V. Chernyshev, A. A. Korlyukov, G. I. Nikishin, A. O. Terent'ev, I. V. Alabugin “Stereo-electronic 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: Stereo-electronic 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 “Stereo-electronic 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[§], **G. P. Gomes[§]**, 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, “Stereo-electronic 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*)

PATENTS

01. R. Pollice, P. Friederich, C. Lavigne, **G. P. Gomes**, A. Aspuru-Guzik “Organic Molecule Light Emitters with High Internal Quantum Efficiency, Low Triplet Population and Fast Reverse Intersystem Crossing for Optoelectronic Applications”, *patent applied*

HONORS & MEDIA

1. Featured on the “*Next Great Impossible*” series by Merck/Milipore-Sigma ([link](#)) 2020
2. *LatinXChem* featured on C&En News ([link](#)) 2020
3. One of the winner teams with “Robo-boat for oil spill management” on *PuebloScience's* Hackathon for Science Education @ UofT, Toronto, ON 2019
4. Featured on Florida State University's College of Arts & Sciences' Spectrum Magazine with the article “*Scientific Sensation*” 2019
5. Selected for IUPAC's Periodic Table of Younger Chemists as “Yttrium” 2018

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| 6. Featured as a Florida State University Student Star | 2018 |
| 7. Florida State University Fellows Society (<i>inducted</i>) | 2017 |
| 8. FSU Student Employee of the Year Award (<i>nomination</i>) | 2017 |
| 9. Honorable Mention: XXXII <i>Jornada Giulio Massarani de Iniciação Científica</i> , as a CNPq Scholar | 2010 |

RESEARCH & WORK EXPERIENCE

- Postdoctoral Researcher at UofT, Aspuru-Guzik Group 2019 – *present*
 - AI for Catalysis, Reaction Discovery, and Optimization. Autonomous Labs.
 - Development of platforms for the inverse-design of catalysts and energy materials.
- Research Assistant (RA) at FSU, Alabugin Group 2014 – 2018
 - Computational and Physical Organic Chemistry.
 - Extensive work on the study and control of chemical reactions with stereoelectronic effects.
- Internship at (Center for Structural Chemistry) CQE-FCUL, Advisor: Dr. Maria José Lourenço 2012 – 2013
 - “Development of electrodes with reduced graphene oxide”
- Undergraduate researcher at INTERLAB-IQ/UFRJ, Advisor: Prof. Pierre Mothé Esteves
- PRH01-ANP scholar, undergrad thesis: “Development and Molecular Study of Methane Hydrates Inhibitors” 2010 – 2012
- CNPq scholar, computational chemist: “Theoretical Study of Electrophilic Aromatic Nitration” 2008 – 2010
- CERN’s GISELA-GRID at IF/UFRJ 2012
 - High performance computing (HPC) manager and infrastructure administrator

MENTORING EXPERIENCE

- Mentor to Graduate Students:
 - Cher-Tian Ser (UofT, 2020 –): “Inverse-designing Suzuki-coupling catalysts with machine-learning”
 - Riley Hickman (UofT, 2019 –): “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 –): “Finding new OLED materials with high-throughput screening”
co-mentored with Dr. Robert Pollice
 - Lucinda Zhu (UofT, 2020 –): “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 – 15): “Computational Studies of Triple-Cycloadditions of Arynes 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*, 3rd 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

- “Mapping the Property Space of Monodentate Organophosphorus Ligands for Catalysis”
invited seminar @ Fordham University, New York City, NY (2021) – to be delivered virtually

2. "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) – to be delivered virtually
3. "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) – *to be delivered virtually*
4. "Mapping the Property Space of Monodentate Organophosphorus Ligands for Catalysis", Aspuru-Guzik Group Meeting @ University of Toronto, Toronto, ON (2021) – *delivered virtually*
5. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Heidelberg Institute for Theoretical Studies, Germany (2020) – *delivered virtually*
6. "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*
7. "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*
8. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Department Seminar @ UFSCar, SP, Brazil (2020) – *delivered virtually*
9. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Tormena Group Meeting @ UNICAMP, SP, Brazil (2020) – *delivered virtually*
10. "Machine Learning Dihydrogen Activation in the Chemical Space Surrounding Vaska's Complex", *invited seminar*, Duarte Group Meeting @ Oxford University, UK (2020) – *delivered virtually*
11. "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*
12. "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*
13. "Computational strategies for learning how to control chemical reactivity", *invited seminar @ Rice University, Houston, TX (2020) – canceled due to COVID-19 travel restrictions*
14. "Computational strategies for learning how to control chemical reactivity", *invited seminar @ University of Houston, Houston, TX (2020) – canceled due to COVID-19 travel restrictions*
15. "Computational strategies for learning how to control chemical reactivity", *invited seminar @ Southern Methodist University, Dallas, TX (2019)*
16. "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)
17. "Machine Learning Reactivity in the Chemical Space of Vaska's Complex", 47th Physical Organic Minisymposium (POMS) @ York University, Toronto, ON (2019)
18. "Computational strategies for learning how to control chemical reactivity", *invited seminar @ Iowa State University, Ames, IA (2019)*
19. "Computational strategies for learning how to control chemical reactivity", *invited seminar @ CINVESTAV, Mexico City, Mexico (2019)*
20. "Computational strategies for learning how to control chemical reactivity", *invited seminar @ UNAM, Mexico City, Mexico (2019)*
21. "Drawing Catalytic Power from Charge Separation: Stereoelectronic and Zwitterionic Assistance in the Au(I)-Catalyzed Bergman Cyclization", ACS COMP Awards poster presentation @ 256th ACS Meeting, Boston, MA (2018)
22. "Taming Oxygen-Rich Systems with Stereoelectronic Effects", oral presentation @ 256th ACS Meeting, Boston, MA (2018)
23. "Drawing Catalytic Power from Charge Separation: Stereoelectronic and Zwitterionic Assistance in the Au(I)-Catalyzed Bergman Cyclization", poster presentation @ CAS, Columbus, OH (2018)
24. "Taming Oxygen-Rich Systems with Stereoelectronic Effects", oral presentation @ Graduate Research Symposium, Indiana University, Bloomington, IN (2018)
25. "Taming Oxygen-Rich Systems with Stereoelectronic Effects", *invited seminar @ Institute of Chemistry, Federal University of Rio de Janeiro, RJ, Brazil (2018)*

26. "Taming Oxygen-Rich Systems with Stereoelectronic Effects", *invited seminar* @ Doyle Group, Princeton University, Princeton, NJ (2018)
27. "Taming Oxygen-Rich Systems with Stereoelectronic Effects", *invited seminar* @ Aspuru-Guzik Group, Harvard University, Cambridge, MA (2018)
28. "Taming Peroxides with Stereoelectronic Effects: Stereoelectronic Control in the Ozone-Free Synthesis of Ozonides", oral presentation, 4th year-talk @ FSU Organic Seminar, Tallahassee, FL (2018)
29. "Taming Peroxides with Stereoelectronic Effects: Stereoelectronic Control in the Ozone-Free Synthesis of Ozonides", poster presentation @ FloHet 2018, Gainesville, FL (2018)
30. "Reinventing cycloaromatization reactions: the diradical/zwitterion dichotomy", [I. V. Alabugin](#), G. P. Gomes @ WATOC 2017, Munich, Germany (2017)
31. "Supramolecular Effects in Radical Chemistry", poster presentation @ 253rd ACS Meeting, San Francisco, CA (2017)
32. "Employing stereoelectronic effects to design organocatalyzed S→F exchange towards functional polythioethers", *invited seminar* @ IBM Research Center, Almaden, CA (2016)
33. "Designing Cascade Cyclizations and Fragmentations with Stereoelectronic Effects: Controlling Radical Arrival and Departure", *invited seminar* @ Todd Martinez Group, Stanford University, CA (2016)
34. "Stereoelectronic effects are in control of reactivity", poster presentation @ SETCA (2016)
35. "Stereoelectronic effects are in control of reactivity", oral presentation, 2nd year-talk @ FSU Organic Seminar, Tallahassee, FL (2016)
36. "Stereoelectronic effects are in control of reactivity", oral presentation @ 92nd FAME, (2016)
37. "Stereoelectronic effects are in control: from the anomalous stability of bis-peroxides to radical cascade cyclizations", poster presentation @ 251th ACS Meeting, San Diego, CA (2016)
38. Computational Design of New Routes to Graphene Nanoribbons, poster presentation @ FSU Digitech (2015)
39. "Theoretical Study of Electrophilic Aromatic Nitration", poster presentation @ XV SBQt (2009)
40. XXXI, XXXII and XXXIV Jornada Giulio Massarani de Iniciação Científica, oral presentations (2009 – 2013)

WORKSHOPS, SYMPOSIUMS & CONFERENCES

41. Workshop: "*Materials Acceleration Platforms: AI, Robotics and Computation for Accelerated Discovery*" @ University of Toronto, Toronto, ON (2020)
42. MolSSI Workshop: Machine Learning and Chemistry: Challenges on the Way Forward @ University of Maryland, College Park, VA (2019)
43. International Meeting on Artificial Intelligence and its Applications (RIIAA @ MEX 2.0), Mexico City, Mexico (2019)
44. DARPA Accelerated Materials Discovery Kick-Off Meeting, Arlington, VA (2019)
45. CAS SciFinder Future Leaders Program @ Columbus, OH (2018)
46. Machine Learning in Science and Engineering Symposium @ Carnegie Mellon University, Pittsburgh, PA (2018)
47. MLx18: A Machine Learning Conference at Florida State University, FSU, Tallahassee, FL (2018)
48. 67th Lindau Nobel Laureate Meeting (Chemistry), Lindau, Germany (2017)
49. Q-Chem 5.0 User Workshop, San Francisco, CA (2017)
50. 24th Winter Inter-American Photochemical Society Conference (2015)
51. School of Advanced Characterization of Nanomaterials of INMETRO (2014)
52. pDynamo Workshop & Molecular Simulation (2013) at University of Sao Paulo, SP – Brazil
53. 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 1st edition ([link](#))
 - ▶ featured on: • *C&EN News*; • *UNICAMP News*
- Reviewer for the 1st Global Inorganic Discussion Weekday Virtual Poster Competition (#gidw2020, [link](#))
- Ongoing peer reviewer for: *ACS Catalysis*, *Journal of Cheminformatics*, *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)

PROGRAMMING, SKILLS & SOFTWARES

- Package development: • *iacta* ([link](#)); • *xtb-gaussian wrapper* ([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