

# Gabriel dos Passos Gomes

• gabriel.gomes@utoronto.ca • (850)-320-3081 • gabegomes.me • 40 St. George Street, Toronto, ON, M5S3H6, Canada

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## EDUCATION & TRAINING

- University of Toronto** (UofT), Department of Chemistry Toronto, ON, Canada
- Postdoctoral Research Fellow, Advisor: Professor Alán Aspuru-Guzik 2019 – *present*
- Florida State University** (FSU), Department of Chemistry and Biochemistry Tallahassee, FL, USA
- PhD Candidate in Chemistry, GPA 4.0, Advisor: Professor Igor V. Alabugin 2014 – 2018
    - *in-flight* MSc in Chemistry 2014 – 2016
- Federal University of Rio de Janeiro** (UFRJ), Institute of Chemistry Rio de Janeiro, RJ, Brazil
- BSc in Chemistry, with technological attributions 2008 – 2013
    - *Science without Borders* scholar, academic exchange at **University of Lisbon** (UL), Portugal 2012 – 2013

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## AWARDS, GRANTS & HONORS

- Featured as a Florida State University Student Star (2018)
- Selected for IUPAC's Periodic Table of Younger Chemists as "Yttrium" (2018)
- CAS SciFinder Future Leaders Program (2018; featured on: • C&EN News; • CAS Program for the 256<sup>th</sup> ACS National Meeting)
- ACS Graduate Research Symposium @ Indiana University, Bloomington, IN (*invited talk*, 2018)
- ACS COMP Chemical Computing Group Excellence Award (2018)
- Machine Learning in Science and Engineering Symposium @ Carnegie Mellon University, Pittsburgh, PA (*travel award*, 2018)
- FSU's Graduate Student Research and Creativity Award (2018)
- Florida State University Fellows Society (*inducted*, 2017)
- 67<sup>th</sup> Lindau Nobel Laureate Meeting (Chemistry), *invitation as young researcher* (2017; featured on:
  - FSU News; • Brazilian Academy of Sciences; • Süddeutsche Zeitung, a German newspaper)
- Philip Schlenoff Graduate Travel Award (2017): grant used to attend the 67<sup>th</sup> Lindau Nobel Laureate Meeting
- FSU Student Employee of the Year Award, *nomination* (2017)
- IBM PhD Scholarship (2016, featured on: • chem.fsu.edu/news; • FSU's Office of Graduate Fellowships and Awards)
- NSF XSEDE (TG-CHE160006): grant in the form of supercomputer time (2016, *renewed* for 2017 & 2018)
- Dr. Martin Luther King Jr. Book Stipend (2016)
- FSU's Congress of Graduate Students (COGS): grant to attend the 253<sup>rd</sup> ACS National Meeting (2016)
- Latin America-Caribbean (LAC) FSU Scholarship (2015 - present)
- Latin American Student Education and Research (LASER) Program Fellowship @ FSU (2014)
- Science without Borders Program and Scholarship @ UL (2012-2013)
- Gas Exploitation Oral Section winner: 6<sup>th</sup> Brazilian Meeting of R&D in Oil and Gas, as PRH01-ANP Scholar (2011)
- Honorable Mention: XXXII Jornada Giulio Massarani de Iniciação Científica, as a CNPq Scholar (2010)

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## PUBLICATIONS (§ = authors contributed equally to this work)

- 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?", *submitted*, **2019**, preprint on ChemRxiv
- 30. A. Hughes, G. P. Gomes**, I. V. Alabugin, "Stereoelectronic Influence of a "Spectator" Propargylic Substituent Can Override Aromaticity Effects in Radical *Peri*-cyclizations on Route to Expanded Polyaromatics", *J. Org. Chem.*, **2019**, *in print*, doi: 10.1021/acs.joc.8b02779
- 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
- 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 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 Stereoelectronic Chameleons: The Donor-Acceptor Dichotomy in Radical Additions", *J. Am. Chem. Soc.*, **2018**, *140* (43), 14272, preprint on ChemRxiv
26. I. V. Alabugin, **G. P. Gomes**, M. Abdo, "Hyperconjugation", *WIREs Comput Mol Sci.*, **2018**;e1389, doi.org/10.1002/wcms.1389
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, doi: 10.1142/9781786344090\_0015
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, Benzanthrenes, 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. 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 "Stereoelectronic 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. Hurtle, 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 as: • *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*-alkenylarylonitriles 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 "Stereoelectronic 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: Stereoelectronic 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 "Stereoelectronic 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*, doi: 10.1002/chem.201781461)

9. 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
8. 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*)
7. E. Berry<sup>s</sup>, **G. P. Gomes**<sup>s</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
6. 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
5. **G. P. Gomes**, V. A. Vil', A. Terent'ev and I. V. Alabugin, "Stereoelectronic 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)
4. 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
3. 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,
2. 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
1. 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: • *amphoterios.com*)

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## RESEARCH, TEACHING, & WORK EXPERIENCE

- Postdoctoral Researcher at UofT (2019-present): Autonomous Labs & Reaction Discovery, Aspuru-Guzik Group
- Reviewer for: *Chemical Science*, *ChemistrySelect*, *ACS Omega*
- Research Assistant (RA) at FSU (2014-2018): Computational Chemistry, Alabugin Group
- Teaching Assistant (TA) at FSU (2015-2017): Organic Chemistry II: Laboratory & Recitation.
- Supervisor to Undergraduate Students:
  - Shelby Davis (Honors Thesis, 2018) "Weaving Together Alkynes to Form Fully Six-Membered Polyaromatic Frameworks"
  - Nicholas Bigerton (Directed Individual Study, 2014-15) "Computational Studies of Triple-Cycloadditions of Arynes to Ynolates"
- Internship at CCMM-FCUL (2013): "Development of electrodes with reduced graphene oxide" Advisor: Dr. M. J. Lourenço
- PRH01-ANP scholar at INTERLAB-IQ/UFRJ (2010-2012): Undergraduate Thesis "Development and Molecular Study of Methane Hydrates Inhibitors". Advisor: Prof. Pierre Esteves
- CERN's GISELA-GRID at IF/UFRJ (2012): High performance computing (HPC) manager and infrastructure administrator.
- Teaching Assistant at *descomplica.com.br*, 3<sup>rd</sup> most innovative company of Latin America by *Fast Company* (2010-2014)
- Teaching Assistant at Institute of Chemistry, UFRJ (2010): Exptl. Organic Chemistry I and II
- CNPq scholar at INTERLAB-IQ/UFRJ (2008-2010): "Theoretical Study of Electrophilic Aromatic Nitration" Dr. Pierre Esteves

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## CONFERENCES, PRESENTATIONS & SERVICE

- "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)
- "Taming Oxygen-Rich Systems with Stereoelectronic Effects", oral presentation @ 256<sup>th</sup> ACS Meeting, Boston, MA (2018)
- "Drawing Catalytic Power from Charge Separation: Stereoelectronic and Zwitterionic Assistance in the Au(I)-Catalyzed Bergman Cyclization", poster presentation @ CAS, Columbus, OH (2018)
- CAS SciFinder Future Leaders Program @ Columbus, OH (2018)
- "Taming Oxygen-Rich Systems with Stereoelectronic Effects", oral presentation @ Graduate Research Symposium, Indiana University, Bloomington, IN (2018)

- “Taming Oxygen-Rich Systems with Stereoelectronic Effects” (*invited talk*), oral presentation @ Institute of Chemistry, Federal University of Rio de Janeiro, RJ, Brazil (2018)
- Machine Learning in Science and Engineering Symposium @ Carnegie Mellon University, Pittsburgh, PA (2018)
- “Taming Oxygen-Rich Systems with Stereoelectronic Effects”, oral presentation @ Doyle Group, Princeton University, Princeton, NJ (2018)
- “Taming Oxygen-Rich Systems with Stereoelectronic Effects”, oral presentation @ Aspuru-Guzik Group, Harvard University, Cambridge, MA (2018)
- “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)
- MLx18: A Machine Learning Conference at Florida State University, FSU, Tallahassee, FL (2018)
- “Taming Peroxides with Stereoelectronic Effects: Stereoelectronic Control in the Ozone-Free Synthesis of Ozonides”, poster presentation @ FloHet 2018, Gainesville, FL (2018)
- “Reinventing cycloaromatization reactions: the diradical/zwitterion dichotomy”, Igor V. Alabugin, Gabriel Gomes @ WATOC 2017, Munich, Germany (2017)
- 67<sup>th</sup> Lindau Nobel Laureate Meeting (Chemistry), Lindau, Germany (2017)
- “Supramolecular Effects in Radical Chemistry”, poster presentation @ 253<sup>rd</sup> ACS Meeting, San Francisco, CA (2017)
- Q-Chem 5.0 User Workshop, San Francisco, CA (2017)
- FSU’s Dr. Martin Luther King Jr. Book Stipend Selection Committee, *invited* (2017)
- “Employing stereoelectronic effects to design organocatalyzed S→F exchange towards functional polythioethers” oral presentation @ IBM Research Center, Almaden, CA (2016)
- “Designing Cascade Cyclizations and Fragmentations with Stereoelectronic Effects: Controlling Radical Arrival and Departure” oral presentation @ Todd Martinez Group, Stanford University, CA (2016)
- “Stereoelectronic effects are in control of reactivity”, poster presentation @ SETCA (2016)
- “Stereoelectronic effects are in control of reactivity”, oral presentation, 2<sup>nd</sup> year-talk @ FSU Organic Seminar, Tallahassee, FL (2016)
- “Stereoelectronic effects are in control of reactivity”, oral presentation @ 92<sup>nd</sup> FAME, (2016)
- “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)
- Graduate Student Commission for Invited Lectures at FSU Dept. of Chemistry and Biochemistry (2016 – 2017)
- Computational Design of New Routes to Graphene Nanoribbons, poster presentation @ FSU Digitech (2015)
- 24<sup>th</sup> Winter Inter-American Photochemical Society Conference, poster presentation (2015)
- School of Advanced Characterization of Nanomaterials of INMETRO (2014)
- pDynamo Workshop & Molecular Simulation (2013) at University of Sao Paulo, SP – Brazil
- School of Advanced Studies in Applied Thermodynamics: Monte Carlo Simulations (2011)
- “Theoretical Study of Electrophilic Aromatic Nitration”, poster presentation @ XV SBQ<sup>t</sup> (2009)
- XXXI, XXXII and XXXIV Jornada Giulio Massarani de Iniciação Científica, oral presentations (2009-2013)
- 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)

## SKILLS & SOFTWARES

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| <ul style="list-style-type: none"> <li>▪ Quantum-Chemical Computations: Gaussian, Jprogdyn, ORCA, Psi4, GFN-xTB, TeraChem, Spartan, Q-Chem</li> <li>▪ Analysis: NBO, NICS-xy, SAPT, ACID, FOD, Aroma</li> <li>▪ Visualization: GaussView, ChemCraft, CYLView, Chimera, PyMol, Jmol</li> </ul> | <ul style="list-style-type: none"> <li>▪ MATLAB, Mathematica, Prism</li> <li>▪ <i>bash</i>, Python</li> <li>▪ Office, Adobe &amp; ChemDraw Suites</li> <li>▪ <u>COP: A Computational Organic Chemistry Routine Parser</u>, developed by G. P. Gomes &amp; D. R. Nascimento @ FSU</li> </ul> |
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## REFERENCES

*Provided upon request.*