

# Carlos H. Borca, Ph.D. | Résumé

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## Computational Chemist | Physics-Based and Machine-Learning Modeling | Bridging Physical Chemistry, AI, and Strategic Analytics

Scientific specialist with 7+ years of experience translating complex modeling, AI, and simulation tools into actionable insights for physical and life sciences and drug discovery teams. Proven ability to communicate technical value, drive software adoption, and support cross-functional stakeholders across science and business. Strong record of impact via peer-reviewed publications, patents, software, and scientific talks.

## Experience

### Industry

- 🔗 DeepCure AI | Boston, MA, USA (Remote) | Role: Principal Scientist – Computational Chemistry (PB/ML Group) 1/2024 – 4/2025
  - 🔗 Led compound selection strategy, aligning physics-based modeling insights with medicinal chemistry goals to accelerate candidate progression
  - 🔗 Designed high-value virtual candidates for a flagship discovery program, leveraging in-house platform capabilities to deliver several confirmed actives
  - 🔗 Enhanced platform performance by integrating physics-based modeling and machine learning, increasing scientific credibility and user adoption
  - 🔗 Evolved virtual screening by implementing advanced electronic structure methods for noncovalent interactions, directly impacting compound triaging
- 🏢 PTC Therapeutics Inc. | Bridgewater, NJ, USA (Hybrid) | Role: Scientist II – Computational Chemistry (CADD Group) 10/2021 – 12/2023
  - 🔗 Led physics-based modeling for RNA-targeted discovery, translating complex simulations into actionable insights for medicinal chemistry
  - 🔗 Accelerated small-molecule design using ligand-based screening, docking, MD, quantum chemistry, and ML-based QSAR modeling
  - 🔗 Developed automated workflows and modeling tools that expanded software utility and improved team efficiency in compound design
  - 🔗 Served as subject-matter expert in collaborations with external partners, aligning computational deliverables with project needs
  - 🔗 Directed cross-functional cloud strategy to support scalable CADD operations, enabling seamless access to high-performance computing
  - 🔗 Optimized in-house compute infrastructure, reducing bottlenecks and boosting scientific throughput for simulation-heavy workflows

### Postdoctoral Research

- 🏠 Princeton University | Princeton, NJ, USA | Adviser: Prof. Michael A. Webb 4/2020 – 9/2021
  - 🔗 Developed quantum-mechanically enriched descriptors to support machine learning-guided polymer design
  - 🔗 Designed a patented AI-driven method to produce chondroitinase ABC/polymer complexes to support sustained neural regeneration
  - 🔗 Pioneered a closed-feedback loop combining robotic polymer-protein fabrication with Bayesian optimization and active learning
  - 🔗 For my work, I was awarded \$10,000 in Azure cloud computing credits by Princeton's Center for Statistics and Machine Learning
- 🏠 Georgia Institute of Technology | Atlanta, GA, USA | Adviser: Prof. C. David Sherrill 9/2017 – 3/2020
  - 🔗 Applied innovative theory for efficient and accurate calculation of crystal lattice energies in pleasantly parallel software
  - 🔗 Led the high-performance computing of extremely accurate benchmark databases of crystal lattice energies for small molecules
  - 🔗 Modeled the self-assembly of non-bonded polymers of hexameric arrays of synthetic nucleobases using molecular dynamics
  - 🔗 Supported and maintained hardware for the Sherrill Group, including building a file system server, multiple workstations, etc.

### Research in Academia and National Laboratories

- 🏫 Purdue University | West Lafayette, IN, USA | Adviser: Prof. Lyudmila V. Slipchenko 2012 – 2017
  - 🔗 Leveraged molecular modeling to enhance the mechanistic design of polymers for pharmaceutical formulations
  - 🔗 Improved the efficiency of polarizable force fields for molecular dynamics by implementing multi-step algorithms
  - 🔗 Explored charge-transfer effects in carbon-based materials for supercapacitors via ground-state density functional theory
  - 🔗 Significantly contributed to support and maintain the Slipchenko Group productivity through system administration duties
- 🎓 Northwestern University | Evanston, IL, USA | Collaborators: Profs. Martín A. Mosquera, Mark A. Ratner, and George C. Schatz 2015 – 2020
  - 🔗 Developed long-range corrections and fragmentation schemes for excitation energy predictions via density functional theory
- 🏢 Lawrence Livermore National Laboratory | Livermore, CA, USA | Advisers: Drs. Alfredo A. Correa and Xavier I. Andrade 2015
  - 🔗 Implemented modular software in C to apply the Tkatchenko-Scheffler density functional correction for van der Waals interactions
- 🎓 Universidad Icesi | Cali, Valle del Cauca, Colombia | Adviser: Prof. Carlos A. Arango 2011 – 2012
  - 🔗 Ran molecular dynamics of water absorbent polymer materials and maintained the Theoretical Chemistry Group's hardware
- 🎓 Universidad del Valle | Cali, Valle del Cauca, Colombia | Adviser: Prof. Julio C. Arce 2007 – 2009
  - 🔗 Simulated interactions of carbon nanotube/DNA hybrids with small molecules for chemical sensing applications

### Peer Reviewing

- International Journal of Pharmaceutics | ScienceDirect | 5 manuscripts 2020 – 2025
- Frontiers in Genetics, Computational Genomics | Frontiers | 1 manuscript 2023
- Journal of Physical Chemistry A | American Chemical Society | 5 manuscripts 2020 – 2022
- Molecular Simulation | Taylor & Francis | 1 manuscript 2021
- Advanced Theory and Simulations | Wiley | 2 manuscript 2019
- The Journal of Chemical Physics | American Institute of Physics | 2 manuscripts 2018 – 2019

## Mentoring

Postgraduate Mentor   Princeton University   Princeton, NJ, USA   2 Graduates	2020 – 2021
Postgraduate Mentor   Georgia Institute of Technology   Atlanta, GA, USA   1 Graduate and 1 Undergraduate	2017 – 2020
Graduate Mentor   Purdue University   West Lafayette, IN, USA   2 Undergraduates	2015 – 2017








## Teaching

Graduate Teaching Assistant   Purdue University   West Lafayette, IN, USA   Computational Chemistry & General Chemistry	2012 – 2015
Laboratory Lecturer   Universidad Icesi   Cali, Valle del Cauca, Colombia   Physical Chemistry I, II, & General Chemistry	2009 – 2011

## Selected Outreach Education Programs and Initiatives

ACS National Chemistry Week 2018   Atlanta, GA, USA   Outreach Volunteer for the Georgia Section	2018
Clubes de Ciencia   Puerto Triunfo, Antioquia, Colombia   Computational Chemistry Science Club Designer and Instructor	2015

## Education

 Postdoctoral Research Associateship	2020 – 2021
Princeton University   Department of Chemical and Biological Engineering   Princeton, NJ, USA	
 Postdoctoral Fellowship	2017 – 2020
Georgia Institute of Technology   School of Chemistry and Biochemistry   Atlanta, GA, USA	
 Ph.D. in Chemistry	2012 – 2017
Purdue University   Department of Chemistry   West Lafayette, IN, USA	
 Applied Management Principles Program   <i>Earned a competitive tuition award from the Department of Chemistry to attend</i> 	2016
Purdue University   Krannert School of Management   West Lafayette, IN, USA	
 Professional Degree in Chemistry (5 Years)   <i>Honors mention for meritorious research thesis</i> 	2004 – 2009
Universidad del Valle   School of Natural and Exact Sciences   Cali, Valle del Cauca, Colombia	

## Languages

Spanish: Native speaker | English: Full professional proficiency (13 years working in the US) | Portuguese: Limited working proficiency

## Computer Skills

Chemistry	Quantum Chemistry	PSI4, Gaussian, Spartan, Q-Chem, Jaguar, Octopus, GAMESS, NWChem, CrystaLattE
	Classical Dynamics	OpenEye, Schrödinger Suite, AMBER, LAMMPS, GROMACS, NAMD, LibEFP/EFPMD
	Molecular Visualization	GaussView, IQmol, VMD, Maestro, PyMol, Avogadro, Gabedit, ChemBioOffice
Online Courses	LinkedIn	Passed skill assessments on Cybersecurity and Linux
	Schrödinger	Intro to Molecular Modeling in Drug Discovery and HTVS for Hit Finding and Evaluation
Scientific Programming	Python, HTML5, C/C++, Fortran	
Data Science & AI/ML	Jupyter, Matplotlib, RDKit, OpenBabel, Keras/TensorFlow, Scikit-Learn, Spyder, ChatGPT, Gemini	
Others	Azure, AWS, LaTeX, GNUPlot, Origin, GitHub, TravisCI, CodeCov, LGTM, Bash, GIMP, Inkscape, LibreOffice	

## Highlighted Honors and Awards


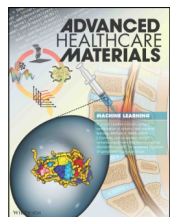
Azure Cloud Computing Credits Grant Award for \$10,000	2020
Center for Statistics and Machine Learning (CSML) at Princeton University   Princeton, NJ, USA	
National Science Foundation Travel Award to attend the CMU-GT Symposium on Machine Learning in Science and Engineering	2018
Carnegie Mellon University   Pittsburgh, PA, USA	
Selected Speaker Honorarium at the Structure and Dynamics in Complex Chemical Systems Symposium	2015
Physical Chemistry Division of the American Chemical Society   Blacksburg, VA, USA	
LLNL Students Poster Symposium Outstanding Accomplishment Award	2015
Lawrence Livermore National Laboratory   Livermore, CA, USA	
Young Scientist and Innovator Scholarship of 2011	2011
Administrative Department of Science, Technology, & Innovation of the Colombian Government (Colciencias) – Cali, Valle del Cauca, Colombia	

## Immigration Status

Legal permanent resident of the United States | Green Card Holder | Dual-citizen of Colombia and Argentina

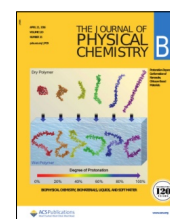
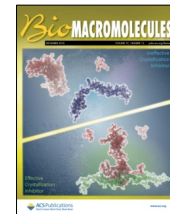
## Peer-reviewed Articles

### Published

25. Carlos H. Borca, Derek P. Metcalf, Zachary L. Glick, Lori A. Burns, and C. David Sherrill. Benchmark Coupled-cluster Lattice Energy of Crystalline Benzene, and Assessment of Multi-level Approximations in the Many-body Expansion. *The Journal of Chemical Physics*, 2023, 158 (23), 234102 DOI: [10.1063/5.0159410](https://doi.org/10.1063/5.0159410)
24. Caroline T. Sargent, Derek P. Metcalf, Zachary L. Glick, Carlos H. Borca, C. David Sherrill. Benchmarking Two-body Contributions to Crystal Lattice Energies and a Range-dependent Assessment of Approximate Methods. *The Journal of Chemical Physics*, 2023, 158 (5) 054112. DOI: [10.1063/5.0141872](https://doi.org/10.1063/5.0141872)
23. Roghayeh Imani, Carlos H. Borca, Meysam Pazoki, and Tomas Edvinsson. Excited-state Charge Polarization and Electronic Structure of Mixed-cation Halide Perovskites: the Role of Mixed Inorganic–organic Cations in CsFAPbI<sub>3</sub>. *RSC Advances*, 2022, 12 (39) 25415–25423. DOI: [10.1039/D2RA04513C](https://doi.org/10.1039/D2RA04513C)
22. Matthew J. Tamasi\*, Roshan A. Patel\*, Carlos H. Borca\*, Shashank Kosuri\*, Heloise Mugnier, Rahul Upadhyay, N. Sanjeeva Murthy, Michael A. Webb, and Adam J. Gormley. Machine Learning on a Robotic Platform for the Design of Polymer–Protein Hybrids. *Advanced Materials*, 2022, 34 (30) 2201809. DOI: [10.1002/adma.202201809](https://doi.org/10.1002/adma.202201809) - Featured in the cover art 
21. Roshan A. Patel, Carlos H. Borca, and Michael A. Webb. Featurization Strategies for Polymer Sequence or Composition Design by Machine Learning. *Molecular Systems Design & Engineering*, 2022, 7 (6) 661–676. DOI: [10.1039/D1ME00160D](https://doi.org/10.1039/D1ME00160D)
20. Shashank Kosuri\*, Carlos H. Borca\*, Heloise Mugnier\*, Matthew Tamasi, Roshan A. Patel, Isabel Perez, Zachary Finkel, Rene Schloss, Li Cai, Martin L. Yarmush, Michael A. Webb, Adam J. Gormley. Machine-Assisted Discovery of Chondroitinase ABC Complexes Towards Sustained Neural Regeneration. *Advanced Healthcare Materials*, 2022, 11 (10) 2102101. DOI: [10.1002/adhm.202102101](https://doi.org/10.1002/adhm.202102101) - Featured in the cover art 
19. Daniel G. A. Smith, Annabelle T. Lolinto, Zachary L. Glick, Jiyoung Lee, Asem Alenaizan, Taylor A. Barnes, Carlos H. Borca, *et al.* Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. *The Journal of Chemical Physics*, 2021, 155 (20) 204801. DOI: [10.1063/5.0059356](https://doi.org/10.1063/5.0059356)
18. Asem Alenaizan, Carlos H. Borca, Suneesh Karunakaran, Amy K. Kendall, Gerald J. Stubbs, Gary B. Schuster, C. David Sherrill, and Nicholas V. Hud. X-ray Fiber Diffraction and Computational Analyses of Stacked Hexads in Supramolecular Polymers: Insight into Self-Assembly in Water by Prospective Prebiotic Nucleobases. *Journal of the American Chemical Society*, 2021, 143, 16, pp 6079–6094. DOI: [10.1021/jacs.0c12010](https://doi.org/10.1021/jacs.0c12010)
17. Venecia R. Wilson, Naila A. Mugheirbi, Laura I. Mosquera-Giraldo, Dana Moseson, Daniel T. Smith, Diana Novo, Carlos H. Borca, Lyudmila V. Slipchenko, Kevin J. Edgar, Lynne S. Taylor. Interaction of Polymers with Enzalutamide Nanodroplets – Impact on Droplet Size and Induction Times. *Molecular Pharmaceutics*, 2021, 18, 3, pp 836–849. DOI: [10.1021/acs.molpharmaceut.0c00833](https://doi.org/10.1021/acs.molpharmaceut.0c00833)
16. Martín A. Mosquera, Leighton O. Jones, Carlos H. Borca, Mark A. Ratner, and George C. Schatz. Domain Separated Density Functional Theory for Reaction Energy Barriers and Optical Excitations. *The Journal of Physical Chemistry A*, 2020, 124 (28) pp 5954–5962. DOI: [10.1021/acs.jpca.0c03596](https://doi.org/10.1021/acs.jpca.0c03596)
15. Nicolas Tancogne-Dejean, Micael J. T. Oliveira, Xavier Andrade, Heiko Appel, Carlos H. Borca, Guillaume Le Breton, *et al.* Octopus, a Computational Framework for Exploring Light-driven Phenomena and Quantum Dynamics in Extended and Finite Systems. *The Journal of Chemical Physics*, 2020, 152 (12) 124119. DOI: [10.1063/1.5142502](https://doi.org/10.1063/1.5142502)
14. Carlos H. Borca, Brandon W. Bakr, Lori A. Burns, and C. David Sherrill. CrystaLattE: Automated Computation of Lattice Energies of Organic Crystals Exploiting the Many-body Expansion to Achieve Dual-level Parallelism. *The Journal of Chemical Physics* 2019, 151 (14) 144103. DOI: [10.1063/1.5120520](https://doi.org/10.1063/1.5120520)
13. Carlos A. Echeverry-Gonzalez, Carlos E. Puerto-Galvis, Carlos H. Borca, Martín A. Mosquera, Andrés F. Luis-Robles, and Vladimir V. Kouznetsov. Optimization of the Synthesis of Quinoline-based Neutral Cyclometalated Iridium Complexes via Microwave Irradiation: Design of Light-harvesting and Emitting Complexes using Bulky Quinolines. *Organic Chemistry Frontiers*, 2019, 6 (19) pp 3374–3382. DOI: [10.1039/C9QO00870E](https://doi.org/10.1039/C9QO00870E)

\*Denotes first co-authorship

12. Tzu-Yen Huang, Felipe A. Larraín, **Carlos H. Borca**, Canek Fuentes-Hernández, Hongping Yan, Sebastian Alexander Schneider, Wen-Fang Chou, Víctor A. Rodríguez-Toro, Hans-Georg Steinrueck, Chuntian Cao, C. David Sherrill, Bernard J. Kippelen, and Michael F. Toney. Morphology of Organic Semiconductors Electrically Doped from Solution Using Phosphomolybdic Acid. *Chemistry of Materials*, 2019, 31 (17) pp 6677–6683. DOI: [10.1021/acs.chemmater.9b01069](https://doi.org/10.1021/acs.chemmater.9b01069)
11. Martín A. Mosquera, Leighton O. Jones, **Carlos H. Borca**, Mark A. Ratner, and George C. Schatz. Fragmentation Schemes Based on Domain Separation in Density Functional Theory. *The Journal of Physical Chemistry A*, 2019, 123 (22) pp 4785–4795. DOI: [10.1021/acs.jpca.9b01173](https://doi.org/10.1021/acs.jpca.9b01173)
10. Laura I. Mosquera-Giraldo, **Carlos H. Borca**, Andrew S. Parker, Yifan Dong, Kevin J. Edgar, Stephen P. Beaudoin, Lyudmila V. Slipchenko, and Lynne S. Taylor. Crystallization Inhibition Properties of Cellulose Ester and Ethers for a Group of Chemically Diverse Drugs - Experimental and Computational Insight. *Biomacromolecules*, 2018, 19 (12), pp 4593–4606. DOI: [10.1021/acs.biomac.8b01280](https://doi.org/10.1021/acs.biomac.8b01280) - Featured in the cover art
9. Naila A. Mugheirbi, Laura I. Mosquera-Giraldo, **Carlos H. Borca**, Lyudmila V. Slipchenko, and Lynne S. Taylor. Phase Behavior of Solid Dispersions Produced using Various Solvent Systems: Mechanistic Understanding of the Role of Polymer using Experimental and Theoretical Methods. *Molecular Pharmaceutics*, 2018, 15 (8), pp 3236–3251. DOI: [10.1021/acs.molpharmaceut.8b00324](https://doi.org/10.1021/acs.molpharmaceut.8b00324)
8. Sarah F. Tyler, Eileen C. Judkins, Dmitry Morozov, **Carlos H. Borca**, Lyudmila V. Slipchenko, and David R. McMillin. To Be or Not to Be Symmetric: That is the Question for Potentially Active Vibronic Modes. *The Journal of Chemical Education*, 2017, 94 (9), pp 1232–1237. DOI: [10.1021/acs.jchemed.7b00289](https://doi.org/10.1021/acs.jchemed.7b00289)
7. Joel D. Rindelaub, **Carlos H. Borca**, Matt A. Hostetler, Mark A. Lipton, Lyudmila V. Slipchenko, and Paul B. Shepson. The Acid-Catalyzed Hydrolysis of an  $\alpha$ -Pinene-Derived Organic Nitrate: Kinetics, Products, Reaction Mechanisms, and Atmospheric Impact. *Atmospheric Chemistry and Physics*, 2016, 16, pp 15425–15432. DOI: [10.5194/acp-2016-726](https://doi.org/10.5194/acp-2016-726)
6. Na Li, Laura I. Mosquera-Giraldo, **Carlos H. Borca**, James D. Ormes, Michael Lowinger, John D. Higgins, Lyudmilla V. Slipchenko, and Lynne S. Taylor. A Comparison of the Crystallization Inhibition Properties of Bile Salts. *Crystal Growth & Design*, 2016, 16 (12) pp 7286–7300. DOI: [10.1021/acs.cgd.6b01470](https://doi.org/10.1021/acs.cgd.6b01470)
5. **Carlos H. Borca**, Lyudmila V. Slipchenko, and Adam Wasserman. Ground-State Charge Transfer: Lithium–Benzene and the Role of Hartree–Fock Exchange. *The Journal of Physical Chemistry A*, 2016, 120 (41) pp 8190–8198. DOI: [10.1021/acs.jpca.6b09014](https://doi.org/10.1021/acs.jpca.6b09014)
4. Laura I. Mosquera-Giraldo, **Carlos H. Borca**, Xiangtao Meng, Kevin J. Edgar, Lyudmilla V. Slipchenko, and Lynne S. Taylor. Mechanistic Design of Chemically Diverse Polymers with Applications in Oral Drug Delivery. *Biomacromolecules*, 2016, 17 (11), pp 3659–3671. DOI: [10.1021/acs.biomac.6b01156](https://doi.org/10.1021/acs.biomac.6b01156)
3. Fulizi Xiong, **Carlos H. Borca**, Lyudmila V. Slipchenko, and Paul B. Shepson. Photochemical Degradation of Isoprene-derived 4,1-Nitrooxy Enal. *Atmospheric Chemistry and Physics*, 2016, 16, pp 5595–5610. DOI: [10.5194/acp-16-5595-2016](https://doi.org/10.5194/acp-16-5595-2016)
2. **Carlos H. Borca** and Carlos A. Arango. Molecular Dynamics of a Water-absorbent Nano-scale Material Based on Chitosan. *The Journal of Physical Chemistry B*, 2016, 120 (15), pp 3754–3765. DOI: [10.1021/acs.jpcb.5b11230](https://doi.org/10.1021/acs.jpcb.5b11230) - Featured in the cover art
1. Martín A. Mosquera, **Carlos H. Borca**, Mark A. Ratner, and George C. Schatz. Connection Between Hybrid Functionals and Importance of the Local Density Approximation. *The Journal of Physical Chemistry A*, 2016, 120 (9), pp 1605–1612. DOI: [10.1021/acs.jpca.5b10864](https://doi.org/10.1021/acs.jpca.5b10864)



## Patents

1. Adam J. Gormley, Matthew Tamasi, Shashank Kosuri, Michael Anthony Webb, **Carlos Hernán Borca Paredes**, Roshan Anit Patel (2024). Method and Systems for a Machine-Assisted Discovery of Chondroitinase ABC Complexes Towards Sustained Neural Regeneration. US Patent US20240355410A1, filed April 25 of 2024, and issued October 24 of 2024.

## Scientific Events

### Events Organized

1. Second Annual Academic Event of the Colombian Student Association at Purdue University | West Lafayette, IN, USA 10/2016  
Head of the academic event organization committee


### Invited Talks

7. Gordon Research Conference on Preclinical Form and Formulation for Drug Discovery | Somerset, VT, USA 6/2023  
Leveraging automation technologies to optimize solutions applicable in the pharmaceutical industry
6. Special Guest Talk at Montana State University's CHMY 513: Computational Chemistry Class | Bozeman, MT, USA 12/2022  
Applications of computational chemistry in the biopharmaceutical industry
5. Special Guest Talk at the George C. Schatz Group Seminar | Evanston, IL, USA 10/2019  
Automated multiscale methods for benchmark-level lattice energies of molecular crystals with CrystaLattE
4. Atlanta Theoretical Chemistry Symposium | Atlanta, GA, USA 9/2019  
CrystaLattE: Automated computation of lattice energies exploiting the many-body expansion to achieve dual-level parallelism
3. Telluride Science Research Center Workshop on Many-Body Interactions: From Quantum Mechanics to Force Fields | Telluride, CO, USA 7/2018  
CrystaLattE: Automated computation of benchmark-level lattice energies of molecular crystals
2. Academic Presentations of the Colombian Student Association at Purdue University | West Lafayette, IN, USA 9/2015  
Developing software to model van der Waals interactions in materials
1. Special Guest Talk at the Graduate Physical Chemistry Seminar at Universidad del Valle | Cali, Valle del Cauca, Colombia 5/2014  
Charge distribution in carbon nanopores via density functional theory




### Contributed Talks

- 22 Latin American Network of Physical Chemistry Theory (RedLatFQT) Webinar | Princeton, NJ, USA 6/2023  
Automated calculation of crystal lattice energies with the many-body cluster expansion
21. 262nd National Meeting & Exposition of the American Chemical Society (ACS Fall 2021) | Atlanta, GA, USA 8/2021  
Smiles4Psi: Automated conformational search with genetic algorithm for quantum-mechanical polymer featurization using Psi4 workflow
20. Virtual Midwest Thermodynamics and Statistical Mechanics Conference (MTSM2021) | Princeton, NJ, USA 6/2021  
Smiles4Psi: Automated conformational search with a genetic algorithm for quantum-mechanical featurization of synthetic polymers
19. Virtual PSI4 World Wide Developers Conference (PsiCon 2020) | Princeton, NJ, USA 12/2020  
Polymer featurization with Psi4 on the Azure cloud
18. 257th National Meeting & Exposition of the American Chemical Society (ACS Spring 2019) | Orlando, FL, USA 4/2019
  - Crystallization inhibition properties of cellulose esters and ethers for a group of chemically diverse drugs
  - Automated multiscale methods for benchmark-level lattice energies of molecular crystals with CrystaLattE
16. 256th National Meeting & Exposition of the American Chemical Society (ACS Fall 2018) | Boston, MA, USA 8/2018  
CrystaLattE: Automated computation of benchmark-level lattice energies of molecular crystals
15. Conference on Machine Learning in Science and Engineering (MLSE 2018) | Pittsburgh, PA, USA 6/2018  
CrystaLattE: Automated computation of benchmark-level lattice energies of molecular crystals 
14. North Carolina State University Building Faculty of the Future Program (NCSU BFF 2018) | Raleigh, NC, USA 3/2018  
CrystaLattE: Automated computation of benchmark-level lattice energies of molecular crystals
13. 47th Meeting of the Southeastern Theoretical Chemistry Association (SETCA 2017) | Oxford, MS, USA 5/2017  
CAM-LDA0: Reincarnating the local density approximation
12. Graduate Physical Chemistry Seminar | West Lafayette, IN, USA 11/2016  
Molecular dynamics with the effective fragment potential method
11. 252th National Meeting & Exposition of the American Chemical Society (ACS Fall 2016) | Philadelphia, PA, USA 8/2016
  - CAM-LDA0: The reincarnation of the local density approximation
  - Timescale separation between energy contributions in the effective fragment potential
  - Molecular dynamics of water-absorbent nanoscale materials based on chitosan



8. 48th Midwest Theoretical Chemistry Conference (MWTCC 2016) | Pittsburgh, PA, USA 6/2016  
Exploiting timescale separation between energy contributions to accelerate molecular dynamics in effective fragment potential
7. Academic Presentations of the Colombian Student Association at Purdue University | West Lafayette, IN, USA 6/2016  
Molecular dynamics of water-absorbent nanoscale materials based on chitosan 
4. 250th National Meeting & Exposition of the American Chemical Society (ACS Fall 2015) | Boston, MA, USA 8/2015
  -  Charge transfer in the lithium–benzene complex via density functional theory
  -  Developing materials-modeling software for electron dynamics with van der Waals interactions 
  -  Determining the melting point of ice with the effective fragment potential
3. V National Meeting of Theoretical and Computational Chemists (V ENQTC) | Guatapé, Antioquia, Colombia 5/2014  
Charge distribution in carbon nanopores via density functional theory
2. IX National Congress of Pure and Applied Chemistry Students (IX CONEQ) | Cali, Valle del Cauca, Colombia 6/2009  
Computational study of interactions between carbon nanotube/DNA hybrids and simple molecules relevant in chemical sensors
1. III National Symposium of Nanotechnology (NANOCOLOMBIA 2009) | Bogotá, D.C., Colombia 4/2009  
Electronic properties of chemical transducers based on carbon nanotubes functionalized with homo-DNA polynucleotides

## Posters

17. 49th Meeting of the Southeastern Theoretical Chemistry Association (SETCA 2019) | Knoxville, TN, USA 5/2019  
CrystaLattE: Automated calculation of lattice energies of organic crystals
16. Institute for Data Engineering and Science Industry Day | Atlanta, GA, USA 3/2018  
CrystaLattE: Automated computation of benchmark-level lattice energies of molecular crystals
15. 49th Midwest Theoretical Chemistry Conference (MWTCC 2017) | East Lansing, MI, USA 6/2017  
CAM-LDA0: Reincarnating the local density approximation
14. 7th Time-Dependent Density-Functional Theory: Prospects and Applications (7th TDDFT) | Benasque, Aragón, Spain 9/2016  
CAM-LDA0: The reincarnation of the local density approximation 
13. IX Congress of the International Society for Theoretical Chemical Physics (IX ISTCP 2016) | Grand Forks, ND, USA 7/2016  
Exploring the Temporal evolution of the energy components in the effective fragment potential molecular dynamics
12. 2016 Conference on Excited State Processes (ESP 2016) | Santa Fe, NM, USA 6/2016  
Charge transfer in the lithium–benzene complex: Understanding the role of the Hartree–Fock exchange
11. Progreso: Research Contributions from Latin America, First Annual Academic Event of the CSAP | West Lafayette, IN, USA 11/2015  
Developing materials-modeling software for electron dynamics with van der Waals interactions
10. Lawrence Livermore National Laboratory Student Poster Symposium | Livermore, CA, USA 7/2015  
Developing materials-modeling software for electron dynamics with van der Waals interactions 
9. 45th Meeting of the Southeastern Theoretical Chemistry Association (SETCA 2015) | Orlando, FL, USA 5/2015  
Charge transfer in lithium–benzene via density functional theory
8. 248th National Meeting & Exposition of the American Chemical Society (ACS Fall 2014) | San Francisco, CA, USA 8/2014  
Charge transfer in lithium–benzene via density functional theory
7. 46th Midwest Theoretical Chemistry Conference (MWTCC 2014) | Evanston, IL, USA 7/2014  
Charge transfer in lithium–benzene via density functional theory
6. VIII National Meeting of Neuroscience | Bogotá, D.C., Colombia 6/2012  
Computational study of glycosylation and phosphorylation of proteins involved in neurodegeneration
5. IV National Meeting of Theoretical and Computational Chemists (IV ENQTC) | Cali, Valle del Cauca, Colombia 5/2012  
Molecular modeling of water absorbent nanoscale materials
4. Fourth Research Socialization Day at Universidad Icesi 2011 | Cali, Valle del Cauca, Colombia 3/2011  
Molecular mechanics study of hydrogel-type biopolymers at the nanoscale 
3. III National Meeting of Theoretical and Computational Chemists (III ENQTC) | San Gil, Santander, Colombia 4/2010  
Electronic response of chemical transducers constituted by carbon nanotubes functionalized with DNA homopolynucleotides
2. XXXV Congress of Theoretical Chemists of Latin Expression (QUITEL 2009) | San Andrés Islas, Colombia 9/2009  
Electronic response of chemical transducers constituted by carbon nanotubes functionalized with DNA homopolynucleotides

1. II National Meeting of Theoretical and Computational Chemists (II ENQTC) | Calarcá, Quindío, Colombia 5/2008  
Computational study of interactions between carbon nanotube/DNA hybrids and simple molecules relevant in chemical sensors

## Participations

18. 18th Drug Discovery Chemistry Conference: Optimizing Small Molecules for Tomorrow's Therapeutics | San Diego, CA, USA 4/2023
17. 5th Annual RNA-Targeted Drug Discovery Conference | Boston, MA, USA 12/2022
16. PTC Therapeutics, Inc. Science Day Forum 2022 | Parsippany, NJ, USA 4/2022
15. 4th Annual RNA-Targeted Drug Discovery Conference (Virtual) | Bridgewater, NJ, USA 12/2021
14. Partnership for an Advanced Computing Environment (PACE) Workshop: Introduction to Deep Learning | Atlanta, GA, USA 6/2020
13. Telluride Science Research Center Virtual Workshop on Many-Body Interactions: Quantum Mechanics to Force Fields | Telluride, CO, USA 6/2020
12. Partnership for an Advanced Computing Environment (PACE) Workshop: Introduction to Machine Learning | Atlanta, GA, USA 11/2019
11. Conference on Machine Learning in Science and Engineering (MLSE 2019) | Atlanta, GA, USA 6/2019
10. PSI4 World Wide Developers Conference (PsiCon 2018) | Atlanta, GA, USA 11/2018
9. Cell Press LabLinks Meeting on Machine Learning in Material and Chemical Sciences at Harvard University | Cambridge, MA, USA 5/2018
8. PSI4 World Wide Developers Conference (PSI4 WWDC 2017) | Blacksburg, VA, USA 11/2017
7. 7th Time-Dependent Density-Functional Theory: Prospects and Applications School and Workshop (7th TDDFT) | Benasque, Aragón, Spain 9/2016
6. 2015 Computational Chemistry and Materials Science Summer Institute (CCMS 2015) | Livermore, CA, USA 6/2015
5. Sustainable Software Innovation Institute for Computational Chemistry and Materials Modeling ((SICM)<sup>2</sup>) | Stony Brook, NY, USA 7/2014
4. II Colombian School on Theory and Computation in Molecular Sciences (II ECTCCM) | Guatapé, Antioquia, Colombia 5/2014
3. 246th National Meeting & Exposition of the American Chemical Society (ACS Fall 2013) | Indianapolis, IN, USA 8/2013
2. 45th Midwest Theoretical Chemistry Conference (MWTC 2013) | Urbana-Champaign, IL, USA 7/2013
1. I Colombian School on Theory and Computation in Molecular Sciences (I ECTCCM) | Cali, Valle del Cauca, Colombia 5/2012

## Other Honors and Awards

- |   |             |
|---|-------------|
| Materials Computational Center Travel Award to attend the 7th TDDFT School and Workshop<br>University of Illinois   Urbana-Champaign, IL, USA   | 2016        |
| Colombian Students Association at Purdue University (CSAP) Travel Grant Award<br>Purdue University   West Lafayette, IN, USA  | 2015        |
| Honors graduation with a mention for meritorious research thesis<br>Universidad del Valle   Cali, Valle del Cauca, Colombia   | 2009        |
| Top-5-in-class academic stimulus scholarship   Six out of eight semesters, including two first places<br>Universidad del Valle   Cali, Colombia   | 2005 – 2008 |
| 11th National ICFES Average Score   Colombian ICFES is analogous to the SAT in the USA, 60,000+ students/year take it<br>Ministry of Education of the Colombian Government   Bogotá, D.C., Colombia | 2004        |
| Andrés Bello Departmental Award for the best Biology score in the ICFES<br>Ministry of Education of the Colombian Government   Bogotá, D.C., Colombia   | 2004        |

## Other Outreach Education Programs and Initiatives

- |   |      |
|---|------|
| Interchange Program 2016   West Lafayette, IN, USA   Theoretical and Computational Chemistry Science Club | 2016 |
| Interchange Program 2015   Medellín, Antioquia, Colombia   Chemistry and Biology Instructor               | 2016 |

## Professional Affiliations

- |   |   |
|---|---|
| American Chemical Society (ACS)                 | Colombian Student Association at Purdue University (CSAP)               |
| Professional Chemists Council of Colombia (CPQ) | Jesuit Alumni Association of Cali, Colombia (A.S.I.A. Santiago de Cali) |

## Personal Interests

- |   |                          |
|---|--------------------------|
| Scale models and computer simulations of aircraft, ships, trains, and automobiles | LEGO                     |
| Electronics repair and upgrade  | Old automobile mechanics |