Carlos H. Borca, Ph.D. | Résumé

☏ +1 (765) 714-3618 • Pennington, New Jersey, USA • Green Card Holder
www.carlosborca.com • www.linkedin.com/in/carlosborca • carlosborca@gmail.com • Google Scholar Profile

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 | *Earned a competitive tuition award from the Department of Chemistry to attend* — 2016
Purdue University | Krannert School of Management | West Lafayette, IN, USA

Professional Degree in Chemistry (5 Years) | *Honors mention for meritorious research thesis* — 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

Addendum

Peer-reviewed Articles

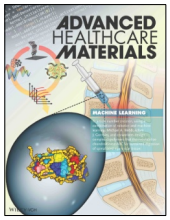
Published

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

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

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 $CsFAPbI_3$. *RSC Advances*, 2022, 12 (39) 25415-25423. DOI: 10.1039/D2RA04513C

22. Matthew J. Tamasi*, Roshan A. Patel*, **Carlos H. Borca***, Shashank Kosuri*, Heloise Mugnier, Rahul Upadhya, 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 - 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

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 - Featured in the cover art

19. Daniel G. A. Smith, Annabelle T. Lolinco, 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

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

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

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

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

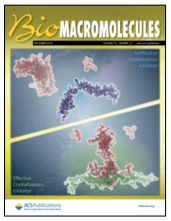
14. **Carlos H. Borca**, Brandon W. Bakr, Lori A. Burns, and C. David Sherrill. CrystaLattE: Automated Computation of Lattice Energies of Organic Crystals Exploiting the Many-body Expansion to Achieve Dual-level Parallelism. The Journal of Chemical Physics 2019, 151 (14) 144103. DOI: 10.1063/1.5120520

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

*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

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



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 - 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

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

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 α-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

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

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

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

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

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 - 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

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-Assissted 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, Quindio, 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)^2) | 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 (MWTCC 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 2016
University of Illinois | Urbana-Champaign, IL, USA

Colombian Students Association at Purdue University (CSAP) Travel Grant Award 2015
Purdue University | West Lafayette, IN, USA

Honors graduation with a mention for meritorious research thesis 2009
Universidad del Valle | Cali, Valle del Cauca, Colombia

Top-5-in-class academic stimulus scholarship | Six out of eight semesters, including two first places 2005 – 2008
Universidad del Valle | Cali, Colombia

11th National ICFES Average Score | Colombian ICFES is analogous to the SAT in the USA, 60,000+ students/year take it 2004
Ministry of Education of the Colombian Government | Bogotá, D.C., Colombia

Andrés Bello Departmental Award for the best Biology score in the ICFES 2004
Ministry of Education of the Colombian Government | Bogotá, D.C., Colombia

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)
Professional Chemists Council of Colombia (CPQ)
Colombian Student Association at Purdue University (CSAP)
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
Electronics repair and upgrade
LEGO
Old automobile mechanics