Carlos H. Borca, Ph.D. | Résumé

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Computational Chemistry Researcher

Molecular Modeling for Biopharmaceutical Applications | Computationally-Aided Materials Design | Computational Chemistry
Data-driven Molecular Design | Active & Deep Learning | Scientific Software Development | Biomacromolecular Simulation | Cloud Computing
Academia & National Laboratories | Multidisciplinary Research | Publications & Presentations | Teaching & Outreach

Experience

Research

Princeton University - Princeton, NJ, USA | Adviser: Prof. Michael A. Webb — 2020 - Present
- Developed deep learning models for data-driven synthesis of polymeric enzyme capsules
- Awarded $10,000 in Azure cloud computing credits by the Microsoft Corporation and the Center for Statistics and Machine Learning
- Simulated the coarse-grained molecular dynamics of ligand-stabilized iron nanoparticles

Georgia Institute of Technology - Atlanta, GA, USA | Adviser: Prof. C. David Sherrill — 2017 - 2020
- Developed of theory and software to compute lattice energies of molecular crystals efficiently and accurately
- Generated benchmark-accuracy databases of lattice energies of molecular crystals
- Analyzed intermolecular interactions of phosphomolybdic acid models with organic polymeric semiconductors
- Modeled self-assembly of non-bonded polymers built by hexameric arrays of synthetic nucleobases

Northwestern University - Evanston, IL, USA | Collaborators: Dr. Martín A. Mosquera, Prof. Mark A. Ratner, and Prof. George C. Schatz — 2015 - 2020
- Informed the design and optimization of light-harvesting and emitting iridium complexes with bulky quinolines
- Designed fragmentation schemes based on domain separation in density functional theory

Purdue University - West Lafayette, IN, USA | Adviser: Prof. Lyudmila V. Slipchenko — 2012 - 2017
- Improved the efficiency of polarizable force fields for molecular dynamics by implementing multi-step algorithms
- Determined the melting temperature of ice modeled with the effective fragment potential method
- Collaborated in the computationally-aided mechanistic design of polymers with applications on pharmaceutics
- Modeled crystallization inhibition properties of bile salts at atomistic scale
- Explored charge-transfer effects in carbon materials for supercapacitors via ground-state density functional theory
- Simulated the photochemical degradation process of isoprene carbonyl nitrates in the atmosphere

Lawrence Livermore National Laboratory - Livermore, CA, USA | Advisers: Dr. Alfredo A. Correa and Dr. Xavier I. Andrade — 2015
- Implemented modular software to apply the Tkatchenko-Scheffler model for van der Waals interactions

Universidad Icesi - Cali, Colombia | Adviser: Prof. Carlos A. Arango — 2011 - 2012
- Conducted atomistic molecular dynamics simulations of water absorbent materials based on chitosan

Universidad del Valle - Cali, Colombia | Adviser: Prof. Julio C. Arce — 2007 - 2009
- Studied interactions of carbon nanotube/DNA hybrids with small molecules for chemical sensing applications

Teaching

Graduate Teaching Assistant | Purdue University - West Lafayette, IN, USA — 2012 - 2015
CHM 57900: Computational Chemistry - Spring 2015
CHM 11100: General Chemistry - Fall 2012, Fall 2013, Fall 2014
CHM 11500: General Chemistry - Spring 2013

Laboratory Lecturer | Universidad Icesi - Cali, Colombia — 2009 - 2011
Physical Chemistry I - 2010-I, 2010-II, 2011-I
Physical Chemistry II - 2010-II
General Chemistry - 2009-II, 2010-I, 2010-II

Mentoring

Postgraduate Mentor (1 Graduate and 1 Undergraduate) | Georgia Institute of Technology - Atlanta, GA, USA — 2017 - 2020

Graduate Mentor (2 Undergraduates) | Purdue University - West Lafayette, IN, USA 2015 - 2017

Outreach Education Programs and Initiatives

ACS National Chemistry Week 2018 - Atlanta, GA, USA | Outreach Volunteer for the Georgia Section 2018

Interchange Program 2016 - West Lafayette, IN, USA | Theoretical and Computational Chemistry Science Club Instructor 2016

Clubes de Ciencia - Colombia 2015 - Puerto Triunfo, Antioquia, Colombia | Computational Chemistry Science Club Designer and Instructor 2015

Interchange Program 2015 - Medellín, Antioquia, Colombia | Chemistry and Biology Instructor 2015

Education

Postdoctoral Research Associateship 2020 - Present
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 Mini-MBA 2016
Purdue University - Krannert School of Management - West Lafayette, IN, USA

Professional (5-Year) Degree in Chemistry | Honors mention for meritorious research thesis 2004 - 2009
Universidad del Valle - School of Natural and Exact Sciences - Cali, Colombia

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)

Languages

Spanish:	Native speaker	
English:	Full professional proficiency	*Live and work in the United States since 2012*
Portuguese:	Limited working proficiency	

Computer Skills

OS:	Linux (Ubuntu, Red Hat, Fedora, CentOS, Cygwin), Windows (98, XP, Vista, 7, 8, 10), and MacOS (Catalina)
Cloud Computing:	Azure
Scientific programming:	Python (NumPy, Jupyter, MatPlotLib, RDKit, OpenBabel, TensorFlow), HTML5, and C/C++
Chemistry:	CrystaLattE, LibEFP/EFPMD, GROMACS, LAMMPS, NAMD, PSI4, Q-Chem, Octopus, GAMESS, HyperChem, Gaussian, MOPAC, NWChem, VMD, IQmol, GaussView, Gabedit, Avogadro, Molden, PyMol, ChemBioOffice
Others:	LaTeX, GNUPlot, Origin, GitHub, TravisCI, CodeCov, LGTM, Bash, GIMP, Inkscape, LibreOffice

Interests

Aircraft, ship, and train models & simulation | Electronics repair & upgrade | LEGO® | Automobile mechanics

Honors and Awards

Azure Cloud Computing Credits Award 2020
Princeton University's Center for Statistics and Machine Learning (CSML) - Princeton, NJ, USA

LLNL Students Poster Symposium Outstanding Accomplishment Award 2015
Lawrence Livermore National Laboratory - Livermore, CA, USA

Eli Lily Scholarship 2014
Purdue University - West Lafayette, IN, USA

Addendum

Peer-reviewed Articles

Under Review

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. *Under Review*, 2021.

Published

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, 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

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

In Preparation (Draft available upon request)

- **Carlos H. Borca** and C. David Sherrill. Multiscale Methods for Benchmark-level Lattice Energies of Molecular Crystals with CrystaLattE. *Manuscript in Preparation*, 2021.
- **Carlos H. Borca** and Lyudmila V. Slipchenko. Exploiting the Timescale Separation between Energy Contributions to Accelerate Molecular Dynamics in the Effective Fragment Potential. *Manuscript in Preparation*, 2021.

Scientific Events

Events Organized

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

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

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

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

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

Virtual PSI4 World Wide Developers Conference (PsiCon 2020) - Princeton, NJ, USA 12/2020
Polymer Featurization with PSI4 on the Azure Cloud

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*

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

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

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

47th Meeting of the Southeastern Theoretical Chemistry Association (SETCA 2017) - Oxford, MS, USA 5/2017
CAM-LDA0: Reincarnating the Local Density Approximation

Graduate Physical Chemistry Seminar - West Lafayette, IN, USA 11/2016
Molecular Dynamics with the Effective Fragment Potential Method

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*

48th Midwest Theoretical Chemistry Conference (MWTCC 2016) - Pittsburgh, PA, USA 6/2016
Exploiting the Timescale Separation between Energy Contributions to Accelerate Molecular Dynamics in the Effective Fragment Potential

Academic Presentations of the Colombian Student Association at Purdue University - West Lafayette, IN, USA 6/2016
Molecular Dynamics of a Water-Absorbent Nanoscale Material Based on Chitosan

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*

V National Meeting of Theoretical and Computational Chemists (V ENQTC) - Guatapé, Antioquia, Colombia 5/2014
Charge Distribution in Carbon Nanopores Via Density Functional Theory

IX National Congress of Pure and Applied Chemistry Students (IX CONEQ) - Cali, Valle del Cauca, Colombia 10/2009
Computational Study of the Interactions between Carbon Nanotube/DNA Hybrids and Simple Molecules Relevant in Chemical Sensing

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

49th Meeting of the Southeastern Theoretical Chemistry Association (SETCA 2019) - Knoxville, TN, USA 5/2019
CrystaLattE: Automated Calculation of Lattice Energies of Organic Crystals

Institute for Data Engineering and Science Industry Day - Atlanta, GA, USA 3/2018
CrystaLattE: Automated Computation of Benchmark-level Lattice Energies of Molecular Crystals

49th Midwest Theoretical Chemistry Conference (MWTCC 2017) - East Lansing, MI, USA 6/2017
CAM-LDA0: Reincarnating the Local Density Approximation

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

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

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

First Annual Academic Event of the Colombian Student Association at Purdue University - West Lafayette, IN, USA 11/2015
Developing Materials-modeling Software for Electron Dynamics with van der Waals Interactions

Lawrence Livermore National Laboratory Student Poster Symposium - Livermore, CA, USA 7/2015
Developing Materials-modeling Software for Electron Dynamics with van der Waals Interactions

45th Meeting of the Southeastern Theoretical Chemistry Association (SETCA 2015) - Orlando, FL, USA 5/2015
Charge Transfer in Lithium-Benzene via Density Functional Theory

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

46th Midwest Theoretical Chemistry Conference (MWTCC 2014) - Evanston, IL, USA 7/2014
Charge Transfer in Lithium-Benzene via Density Functional Theory

VIII National Meeting of Neuroscience - Bogotá, D.C., Colombia 6/2012
Computational Study of Glycosylation and Phosphorylation of Proteins Involved in Neurodegeneration

IV National Meeting of Theoretical and Computational Chemists (IV ENQTC) - Cali, Valle del Cauca, Colombia 5/2012
Molecular Modelling of Water Absorbent Nanoscale Materials

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

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

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

II National Meeting of Theoretical and Computational Chemists (II ENQTC) - Calarcá, Quindio, Colombia 4/2010
Computational Study of the Interactions between Carbon Nanotube/DNA Hybrids and Simple Molecules Relevant in Chemical Sensing

Participations

Partnership for an Advanced Computing Environment (PACE) Virtual Workshop: Introduction to Deep Learning 6/2020
Atlanta, GA, USA

Telluride Science Research Center Virtual Workshop on Many-Body Interactions: Quantum Mechanics to Force Fields 6/2020
Telluride, CO, USA

Partnership for an Advanced Computing Environment (PACE) Workshop: Introduction to Machine Learning 11/2019
Atlanta, GA, USA

Conference on Machine Learning in Science and Engineering (MLSE 2019) 6/2019
Atlanta, GA, USA

PSI4 World Wide Developers Conference (PsiCon 2018) 11/2018
Atlanta, GA, USA

Cell Press LabLinks Meeting on Machine Learning in Material and Chemical Sciences at Harvard University 5/2018
Cambridge, MA, USA

PSI4 World Wide Developers Conference (PSI4 WWDC 2017) 11/2017
Blacksburg, VA, USA

7th Time-Dependent Density-Functional Theory: Prospects and Applications School and Workshop (7th TDDFT) 9/2016
Benasque, Aragón, Spain

2015 Computational Chemistry and Materials Science Summer Institute (CCMS 2015) 6/2015
Livermore, CA, USA

Sustainable Software Innovation Institute for Computational Chemistry and Materials Modeling ($(SICM)^2$) 7/2014
Stony Brook, NY, USA

II Colombian School on Theory and Computation in Molecular Sciences (II ECTCCM) 5/2014
Guatapé, Antioquia, Colombia

246th National Meeting & Exposition of the American Chemical Society (ACS Fall 2013) 8/2013
Indianapolis, IN, USA

45th Midwest Theoretical Chemistry Conference (MWTCC 2013) 7/2013
Urbana-Champaign, IL, USA

IX International Seminar of Neuroscience 6/2012
Bogotá, D.C., Colombia

I Colombian School on Theory and Computation in Molecular Sciences (I ECTCCM) 5/2012
Cali, Valle del Cauca, Colombia