Carlos H. Borca, Ph.D. | Résumé

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Computational Chemistry Researcher

Molecular Modeling for Biopharmaceutical Applications | Computationally-Aided Materials Design | Computational Chemistry Original Scientific Software Development | Deep Learning & Descriptors | Biomacromolecular Structure | *Ab initio* Simulation Academia & National Laboratories | Multidisciplinary Research | Publications & Presentations | Teaching & Outreach

Experience

Experience	
Research	
Princeton University - Princeton, NJ, USA Adviser: Prof. Michael A. Webb O Deep learning methods development for data-driven design of functionalized polymers	020 - Present
Georgia Institute of Technology - Atlanta, GA, USA Adviser: Prof. C. David Sherrill 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	2017 - 2020
Northwestern University - Evanston, IL, USA Collaborators: Dr. Martín A. Mosquera, Prof. Mark A. Ratner, and Prof. George C. Schatz o Informed the design and optimization of light-harvesting and emitting iridium complexes with bulky quinolines o Designed fragmentation schemes based on domain separation in density functional theory o Developed and tested long-range corrected local density functionals for excitation energies	2015 - 2020
Purdue University - West Lafayette, IN, USA Adviser: Prof. Lyudmila V. Slipchenko 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 • Implemented modular software to apply the Tkatchenko-Scheffler model for van der Waals interactions	2015
Universidad Icesi - Cali, Colombia Adviser: Prof. Carlos A. Arango Conducted atomistic molecular dynamics simulations of water absorbent materials based on chitosan	2011 - 2012
Universidad del Valle - Cali, Colombia Adviser: Prof. Julio C. Arce • Studied interactions of carbon nanotube/DNA hybrids with small molecules for chemical sensing applications	2007 - 2009
Teaching. Graduate Teaching Assistant Purdue University - West Lafayette, IN, USA CHM 57900: Computational Chemistry - Spring 2015 CHM 11100: General Chemistry - Fall 2012, Fall 2013, Fall 2014 CHM 11500: General Chemistry - Spring 2013	2012 - 2015
Laboratory Lecturer Universidad Icesi - Cali, Colombia Physical Chemistry I - 2010-I, 2010-II, 2011-I Physical Chemistry II - 2010-II General Chemistry - 2009-II, 2010-I, 2010-II	2009 - 2011
Mentoring	

Postgraduate Mentor | Georgia Institute of Technology - Atlanta, GA, USA

2017 - 2019

Asem Alenaizan - *Graduate Student Researcher in Chemistry* Donna Odhiambo - *Undergraduate Student Researcher in Chemistry*

Graduate Mentor | Purdue University - West Lafayette, IN, USA

2015 - 2017

Jennifer Werner - Undergraduate Student Researcher in Chemistry Yifan Wang - Undergraduate Student Researcher in Chemistry

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

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

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

2018

2018

Education

Postdoctoral Research Associateship Princeton University - Department of Chemical and Biological Engineering - Princeton, NJ, USA	2020 - Present
Postdoctoral Fellowship Georgia Institute of Technology - School of Chemistry and Biochemistry - Atlanta, GA, USA	2017 - 2020
Ph.D. in Chemistry Purdue University - Department of Chemistry - West Lafayette, IN, USA	2012 - 2017
Applied Management Principles Mini-MBA Purdue University - Krannert School of Management - West Lafayette, IN, USA	2016
Professional (5-Year) Degree in Chemistry Honors mention for meritorious research thesis	2004 - 2009

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 (10, 7, Vista, XP, 98), and MacOS (Catalina)

Scientific programing: Python, HTML, C/C++

Chemistry: CrystaLattE, LibEFP/EFPMD, GROMACS, NAMD, PSI4, Q-Chem, Octopus, GAMESS, HyperChem, Gaussian,

MOPAC, NWChem, Molpro, VMD, IQmol, GaussView, Gabedit, Avogadro, Molden, PyMol, ChemBioOffice

Others: Jupyter, धान्X, MatPlotlib, GNUPlot, Origin, Git, Bash, GIMP, Inkscape, Office, LibreOffice

Interests

Aircraft & train models & simulation | Electronics repair & upgrade | LEGO(R) | Automobile mechanics

Honors and Awards

LLNL Students Poster Symposium Outstanding Accomplishment Award

Universidad del Valle - School of Natural and Exact Sciences - Cali, Colombia

Lawrence Livermore National Laboratory - Livermore, CA, USA

Eli Lily Scholarship 2014

Purdue University - West Lafayette, IN, USA

Young Scientist and Innovator Scholarship of 2011

2011

2015

Administrative Department of Science, Technology, and Innovation of the Colombian Government (Colciencias) and Universidad Icesi - Cali, Colombia

Addendum

Peer-reviewed Articles

In Press

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, (In Press), 2020. DOI: 10.1021/acs.jpca.0c03596

Published.....

- 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/C9Q000870E
- 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)

- o Carlos H. Borca and C. David Sherrill. Multiscale Methods for Benchmark-level Lattice Energies of Molecular Crystals with CrystaLattE. Manuscript in Preparation, 2020.
- o Asem Alenaizan, Carlos H. Borca, Nicholas V. Hud, and C. David Sherrill. Noncovalent Interactions in Supramolecular Polymers Based on Hexameric Rosettes of Proto-nucleobases. Manuscript in Preparation, 2020.
- o 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, 2020.

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Scientific Events	
Events Organized	
Second Annual Academic Event of the Colombian Student Association at Purdue University - West Lafayette, IN, USA Head of the Academic Event Organization Committee	10/2016
Invited Talks	
Atlanta Theoretical Chemistry Symposium - Atlanta, GA, USA CrystaLattE: Automated Computation of Lattice Energies Exploiting the Many-body Expansion to Achieve Dual-level Parallelism	9/2019
Telluride Science Research Center Workshop on Many-Body Interactions: From Quantum Mechanics to Force Fields - Telluride, CO, USA CrystaLattE: Automated Computation of Benchmark-level Lattice Energies of Molecular Crystals	7/2018
Academic Presentations of the Colombian Student Association at Purdue University - West Lafayette, IN, USA Developing Software to Model van der Waals Interactions in Materials	9/2015
Special Guest Talk at the Graduate Physical Chemistry Seminar at Universidad del Valle - Cali, Valle del Cauca, Colombia Charge Distribution in Carbon Nanopores Via Density Functional Theory	5/2014
Contributed Talks	
 257th National Meeting & Exposition of the American Chemical Society (ACS Spring 2019) - Orlando, FL, USA 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 	4/2019
256th National Meeting & Exposition of the American Chemical Society (ACS Fall 2018) - Boston, MA, USA CrystaLattE: Automated Computation of Benchmark-level Lattice Energies of Molecular Crystals	8/2018
Conference on Machine Learning in Science and Engineering (MLSE 2018) - Pittsburgh, PA, USA CrystaLattE: Automated Computation of Benchmark-level Lattice Energies of Molecular Crystals	6/2018
North Carolina State University Building Faculty of the Future Program (NCSU BFF 2018) - Raleigh, NC, USA CrystaLattE: Automated Computation of Benchmark-level Lattice Energies of Molecular Crystals	3/2018
47th Meeting of the Southeastern Theoretical Chemistry Association (SETCA 2017) - Oxford, MS, USA CAM-LDAO: Reincarnating the Local Density Approximation	5/2017
Graduate Physical Chemistry Seminar - West Lafayette, IN, USA Molecular Dynamics with the Effective Fragment Potential Method	11/2016
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 Exploiting the Timescale Separation between Energy Contributions to Accelerate Molecular Dynamics in the Effective Fragment Potential	6/2016

Partnership for an Advanced Computing Environment (PACE) Virtual Workshop: Introduction to Deep Learning Atlanta, GA, USA	6/2020
Participations	
II National Meeting of Theoretical and Computational Chemists (II ENQTC) - Calarcá, Quindio, Colombia Computational Study of the Interactions between Carbon Nanotube/DNA Hybrids and Simple Molecules Relevant in Chemical Sensing	4/2010
XXXV Congress of Theoretical Chemists of Latin Expression (QUITEL 2009) - San Andrés Islas, Colombia Electronic Response of Chemical Transducers Constituted by Carbon Nanotubes Functionalized with DNA Homopolynucleotides	9/2009
III National Meeting of Theoretical and Computational Chemists (III ENQTC) - San Gil, Santander, Colombia Electronic Response of Chemical Transducers Constituted by Carbon Nanotubes Functionalized with DNA Homopolynucleotides	4/2010
Fourth Research Socialization Day at Universidad Icesi 2011 - Cali, Valle del Cauca, Colombia Molecular Mechanics Study of Hydrogel-type Biopolymers at the Nanoscale	3/2011
IV National Meeting of Theoretical and Computational Chemists (IV ENQTC) - Cali, Valle del Cauca, Colombia Molecular Modelling of Water Absorbent Nanoscale Materials	5/2012
VIII National Meeting of Neuroscience - Bogotá, D.C., Colombia Computational Study of Glycosylation and Phosphorylation of Proteins Involved in Neurodegeneration	6/2012
Charge Transfer in Lithium-Benzene via Density Functional Theory	•
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 248th National Meeting & Exposition of the American Chemical Society (ACS Fall 2014) - San Francisco, CA, USA	8/2014
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
Lawrence Livermore National Laboratory Student Poster Symposium - Livermore, CA, USA	7/2015
First Annual Academic Event of the Colombian Student Association at Purdue University - West Lafayette, IN, USA Developing Materials-modeling Software for Electron Dynamics with van der Waals Interactions	11/2015
2016 Conference on Excited State Processes (ESP 2016) - Santa Fe, NM, USA Charge Transfer in the Lithium-Benzene Complex: Understanding the Role of the Hartree-Fock Exchange	6/2016
IX Congress of the International Society for Theoretical Chemical Physics (IX ISTCP 2016) - Grand Forks, ND, USA Exploring the Temporal Evolution of the Energy Components in the Effective Fragment Potential Molecular Dynamics	7/2016
7th Time-Dependent Density-Functional Theory: Prospects and Applications (7th TDDFT) - Benasque, Aragón, Spain CAM-LDAO: The Reincarnation of the Local Density Approximation	9/2016
CAM-LDAO: Reincarnating the Local Density Approximation	·
CrystaLattE: Automated Computation of Benchmark-level Lattice Energies of Molecular Crystals 49th Midwest Theoretical Chemistry Conference (MWTCC 2017) - East Lansing, MI, USA	6/2017
CrystaLattE: Automated Calculation of Lattice Energies of Organic Crystals Institute for Data Engineering and Science Industry Day - Atlanta, GA, USA	3/2018
49th Meeting of the Southeastern Theoretical Chemistry Association (SETCA 2019) - Knoxville, TN, USA	5/2019
Posters.	
III National Symposium of Nanotechnology (NANOCOLOMBIA 2009) - Bogotá, D.C., Colombia Electronic Properties of Chemical Transducers Based on Carbon Nanotubes Functionalized with Homo-DNA polynucleotides	4/2009
IX National Congress of Pure and Applied Chemistry Students (IX CONEQ) - Cali, Valle del Cauca, Colombia Computational Study of the Interactions between Carbon Nanotube/DNA Hybrids and Simple Molecules Relevant in Chemical Sensing	10/2009
V National Meeting of Theoretical and Computational Chemists (V ENQTC) - Guatapé, Antioquia, Colombia Charge Distribution in Carbon Nanopores Via Density Functional Theory	5/2014
• Determining the Melting Point of Ice with the Effective Fragment Potential	
 Charge Transfer in the Lithium-Benzene Complex via Density Functional Theory Developing materials-modeling software for electron dynamics with van der Waals interactions 	
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
Academic Presentations of the Colombian Student Association at Purdue University - West Lafayette, IN, USA	6/2016

Telluride Science Research Center Virtual Workshop on Many-Body Interactions: Quantum Mechanics to Force F Telluride, CO, USA	ields 6/2020
Partnership for an Advanced Computing Environment (PACE) Workshop: Introduction to Machine Learning Atlanta, GA, USA	11/2019
Conference on Machine Learning in Science and Engineering (MLSE 2019) Atlanta, GA, USA	6/2019
PSI4 World Wide Developers Conference (PsiCon 2018) Atlanta, GA, USA	11/2018
Cell Press LabLinks Meeting on Machine Learning in Material and Chemical Sciences at Harvard University Cambridge, MA, USA	5/2018
PSI4 World Wide Developers Conference (PSI4 WWDC 2017) Blacksburg, VA, USA	11/2017
7th Time-Dependent Density-Functional Theory: Prospects and Applications School and Workshop (7th TDDFT) Benasque, Aragón, Spain	9/2016
2015 Computational Chemistry and Materials Science Summer Institute (CCMS 2015) Livermore, CA, USA	6/2015
Sustainable Software Innovation Institute for Computational Chemistry and Materials Modeling ((SICM) ²) Stony Brook, NY, USA	7/2014
II Colombian School on Theory and Computation in Molecular Sciences (II ECTCCM) Guatapé, Antioquia, Colombia	5/2014
246th National Meeting & Exposition of the American Chemical Society (ACS Fall 2013) Indianapolis, IN, USA	8/2013
45th Midwest Theoretical Chemistry Conference (MWTCC 2013) Urbana-Champaign, IL, USA	7/2013
IX International Seminar of Neuroscience Bogotá, D.C., Colombia	6/2012
I Colombian School on Theory and Computation in Molecular Sciences (I ECTCCM) Cali, Valle del Cauca, Colombia	5/2012
References	
Prof. Michael A. Webb Postdoctoral Adviser Assistant Professor - Department of Chemical and Biological Engineering - Princeton University Email: mawebb@princeton.edu Office Phone: +1 (609) 258-4595	2020 - Present
Prof. C. David Sherrill Postdoctoral Adviser Professor - Department of Chemistry - Georgia Institute of Technology Email: sherrill@gatech.edu Office Phone: +1 (404) 894-7452	2017 - Present
Prof. Lyudmila V. Slipchenko Doctoral Adviser Professor - Department of Chemistry - Purdue University Email: lslipchenko@purdue.edu Office Phone: +1 (765) 494-5255	2012 - 2018
Prof. Lynne S. Taylor Multidisciplinary Research Collaborator Retter Professor of Pharmacy - Department of Industrial and Physical Pharmacy - Purdue University Email: lstaylor@purdue.edu Office Phone: +1 (765) 496-6614	2014 - 2018