

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 | Machine Learning Descriptors | Biomacromolecular Structure | *Ab initio* Simulation
Academia & National Laboratories | Multidisciplinary Research | Publications & Presentations | Teaching & Outreach

Experience

Research.....

Georgia Institute of Technology - Atlanta, GA, USA | Adviser: Prof. C. David Sherrill 2017 - Present

- Development of theory and software to compute properties of molecular organic crystals
- Generation highly-accurate databases of lattice energies of molecular crystals
- Molecular modeling of self-assembling non-bonded polymers
- Intermolecular interactions of phosphomolybdic acid models and organic polymeric semiconductors
- Computational benchmarking of interactions of molecules with halogen-polarized C-H and aromatic rings

Northwestern University - Evanston, IL, USA | Collaborators: Dr. Martín A. Mosquera, Prof. Mark A. Ratner, and Prof. George C. Schatz 2015 - 2019

- Design and optimization of light-harvesting and emitting iridium complexes using bulky quinolines
- Fragmentation schemes based on domain separation in density functional theory
- Development of long-range corrected local density functionals for excitation energies

Purdue University - West Lafayette, IN, USA | Adviser: Prof. Lyudmila V. Slipchenko 2012 - 2017

- Computationally-aided mechanistic design of polymers with applications on pharmaceuticals
- Molecular modeling of crystallization inhibition properties of bile salts
- Improvement of the computational efficiency of polarizable force fields for molecular dynamics
- Determination of the melting temperature of ice modeled with the effective fragment potential method
- Charge-transfer effects in carbon materials for supercapacitors via ground-state density functional theory
- Simulations on 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

- Modular software implementation of the Tkatchenko-Scheffler model for van der Waals interactions

Universidad Icesi - Cali, Colombia | Adviser: Prof. Carlos A. Arango 2011 - 2012

- Atomistic molecular dynamics simulations of water absorbent materials at the nano-scale

Universidad del Valle - Cali, Colombia | Adviser: Prof. Julio C. Arce 2007 - 2009

- Computational study of interactions of single-wall carbon nanotubes/DNA hybrids and small molecules relevant to 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 | 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
Jennifer Werner - Undergraduate Student Researcher in Chemistry
Yifan Wang - Undergraduate Student Researcher in Chemistry

2015 - 2017

Outreach Education Programs and Initiatives

ACS National Chemistry Week 2018 - Atlanta, GA, USA | Outreach Volunteer for the Georgia Section 2018
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 Fellowship 2017 - Present
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, SUSE, Cygwin.
Windows | 98, XP, Vista, 7, 8, 10.
Basic programming: Python, HTML, C/C++, Fortran.
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: \LaTeX , gnuplot, GIMP, Git, Bash, Origin, Inkscape, Office, LibreOffice, Jupyter.

Interests

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

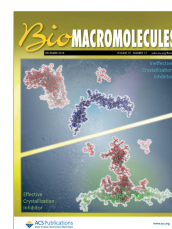
Honors and Awards

Materials Computational Center Travel Award to attend the 7th TDDFT School and Workshop 2016
University of Illinois - Urbana-Champaign, IL, 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
Young Scientist and Innovator Scholarship of 2011 2011
Administrative Department of Science, Technology, and Innovation of the Colombian Government (Colciencias) and Universidad Icesi - Cali, Colombia

Peer-reviewed Articles

Published

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
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.
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
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
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
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
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
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
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
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.
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
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
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



In Press

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 (In Press)*, 2019.

In Preparation (Draft available)

- **Carlos H. Borca** and C. David Sherrill. Multiscale Methods for Benchmark-level Lattice Energies of Molecular Crystals with CrystaLattE. *Manuscript in Preparation*, 2019.
- 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*, 2019.
- Nicolas Tancogne-Dejean, **et. al.** Octopus, a Framework for Exploring Ultrafast Electron Dynamics in Periodic and Isolated Systems. *Manuscript in Preparation*, 2019.
- **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*, 2019.

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

2019 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

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

Machine Learning in Science and Engineering Conference - 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 - 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 <i>Charge Distribution in Carbon Nanopores Via Density Functional Theory</i>	5/2014
IX National Congress of Pure and Applied Chemistry Students (IX CONEQ) - Cali, Valle del Cauca, Colombia <i>Computational Study of the Interactions between Carbon Nanotube/DNA Hybrids and Simple Molecules Relevant in Chemical Sensing</i>	10/2009
III National Symposium of Nanotechnology (NANOCOLOMBIA 2009) - Bogotá, D.C., Colombia <i>Electronic Properties of Chemical Transducers Based on Carbon Nanotubes Functionalized with Homo-DNA polynucleotides</i>	4/2009

Posters

49th Meeting of the Southeastern Theoretical Chemistry Association (SETCA 2019) - Knoxville, TN, USA <i>CrystaLattE: Automated Calculation of Lattice Energies of Organic Crystals</i>	5/2019
Institute for Data Engineering and Science Industry Day - Atlanta, GA, USA <i>CrystaLattE: Automated Computation of Benchmark-level Lattice Energies of Molecular Crystals</i>	3/2018
49th Midwest Theoretical Chemistry Conference (MWTCC 2017) - East Lansing, MI, USA <i>CAM-LDA0: Reincarnating the Local Density Approximation</i>	6/2017
7th Time-Dependent Density-Functional Theory: Prospects and Applications (7th TDDFT) - Benasque, Aragón, Spain <i>CAM-LDA0: The Reincarnation of the Local Density Approximation</i>	9/2016
IX Congress of the International Society for Theoretical Chemical Physics (IX ISTCP 2016) - Grand Forks, ND, USA <i>Exploring the Temporal Evolution of the Energy Components in the Effective Fragment Potential Molecular Dynamics</i>	7/2016
2016 Conference on Excited State Processes (ESP 2016) - Santa Fe, NM, USA <i>Charge Transfer in the Lithium-Benzene Complex: Understanding the Role of the Hartree-Fock Exchange</i>	6/2016
First Annual Academic Event of the Colombian Student Association at Purdue University - West Lafayette, IN, USA <i>Developing Materials-modeling Software for Electron Dynamics with van der Waals Interactions</i>	11/2015
Lawrence Livermore National Laboratory Student Poster Symposium - Livermore, CA, USA <i>Developing Materials-modeling Software for Electron Dynamics with van der Waals Interactions</i>	7/2015
45th Meeting of the Southeastern Theoretical Chemistry Association (SETCA 2015) - Orlando, FL, USA <i>Charge Transfer in Lithium-Benzene via Density Functional Theory</i>	5/2015
248th National Meeting & Exposition of the American Chemical Society (ACS Fall 2014) - San Francisco, CA, USA <i>Charge Transfer in Lithium-Benzene via Density Functional Theory</i>	8/2014
46th Midwest Theoretical Chemistry Conference (MWTCC 2014) - Evanston, IL, USA <i>Charge Transfer in Lithium-Benzene via Density Functional Theory</i>	7/2014
VIII National Meeting of Neuroscience - Bogotá, D.C., Colombia <i>Computational Study of Glycosylation and Phosphorylation of Proteins Involved in Neurodegeneration</i>	6/2012
IV National Meeting of Theoretical and Computational Chemists (IV ENQTC) - Cali, Valle del Cauca, Colombia <i>Molecular Modelling of Water Absorbent Nanoscale Materials</i>	5/2012
Fourth Research Socialization Day at Universidad Icesi 2011 - Cali, Valle del Cauca, Colombia <i>Molecular Mechanics Study of Hydrogel-type Biopolymers at the Nanoscale</i>	3/2011
III National Meeting of Theoretical and Computational Chemists (III ENQTC) - San Gil, Santander, Colombia <i>Electronic Response of Chemical Transducers Constituted by Carbon Nanotubes Functionalized with DNA Homopolynucleotides</i>	4/2010
XXXV Congress of Theoretical Chemists of Latin Expression (QUITEL 2009) - San Andrés Islas, Colombia <i>Electronic Response of Chemical Transducers Constituted by Carbon Nanotubes Functionalized with DNA Homopolynucleotides</i>	9/2009
II National Meeting of Theoretical and Computational Chemists (II ENQTC) - Calarcá, Quindío, Colombia <i>Computational Study of the Interactions between Carbon Nanotube/DNA Hybrids and Simple Molecules Relevant in Chemical Sensing</i>	4/2010

Participations

Machine Learning in Science and Engineering Conference 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. C. David Sherrill <i>Postdoctoral Adviser</i> Professor - Department of Chemistry - Georgia Institute of Technology Email: sherrill@gatech.edu Office Phone: +1 (404) 894-7452	2017 - Present
Prof. Lyudmila V. Slipchenko <i>Doctoral Adviser</i> Associate Professor - Department of Chemistry - Purdue University Email: lslipchenko@purdue.edu Office Phone: +1 (765) 494-5255	2012 - Present
Prof. Lynne S. Taylor <i>Multidisciplinary Research Collaborator</i> Retter Professor of Pharmacy - Department of Industrial and Physical Pharmacy - Purdue University Email: ltaylor@purdue.edu Office Phone: +1 (765) 496-6614	2014 - Present