

Carlos H. Borca, Ph.D. | Résumé

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Computational Chemistry Researcher

Molecular Modeling for Pharmaceutical Applications | Computational Chemistry | Original Scientific Software Development
Computationally-Aided Materials Design | Biomolecular Structure | *Ab initio* Simulation | Machine Learning Descriptors
Academia & National Laboratories | Collaborative 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
- Computational benchmarking of interactions of molecules with halogen-polarized C-H and aromatic rings

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

- 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
- Computationally-aided mechanistic design of polymers with applications on pharmaceuticals
- Molecular modeling of crystallization inhibition properties of bile salts
- Simulations on photochemical degradation process of isoprene carbonyl nitrates in the atmosphere
- Charge-transfer effects in carbon materials for supercapacitors via ground-state density functional theory

Northwestern University - Evanston, IL, USA | Collaborators: Dr. Martín A. Mosquera, Prof. Mark A. Ratner, and George C. Schatz 2015 - 2016

- Development of long-rang corrected local density functionals for excitation energies
- Impact of spherical deformations in the electronic structure of graphene-like molecular models

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 - 2018

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

Interchange Program 2016 - West Lafayette, IN, USA Theoretical and Computational Chemistry Science Club	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 Fellowship Georgia Institute of Technology - School of Chemistry and Biochemistry - Atlanta, GA, USA	2017 - Present
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 Universidad del Valle - School of Natural and Exact Sciences - Cali, Colombia	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:	Fluently spoken and written.	<i>Live and work in the United States since 2012.</i>
Portuguese:	Intermediate proficiency.	

Computer Skills

Chemistry:	LibEFP/EFPM, GROMACS, NAMD, PSI4, Q-Chem, Octopus, GAMESS, HyperChem, Gaussian, MOPAC, NWChem, VMD, IQmol, GaussView, Gabedit, Avogadro, Molden, ChemBioOffice.
OS:	Linux Ubuntu, Red Hat, SUSE, CentOS, Cygwin. Windows 98, XP, Vista, 7, 8, 10.
Basic programming:	Python, HTML, C/C++.
Others:	LaTeX, gnuplot, GIMP, Git, Bash, Origin, Inkscape, Office, LibreOffice, Jupyter.

Interests

Computer repair & upgrade | Aircraft & train modeling & simulation | LEGO® | Automobile mechanics

Honors and Awards

National Science Foundation Travel Award to attend the CMU-GT Symposium on Machine Learning in Science and Engineering Carnegie Mellon University - Pittsburgh, PA, USA	2018
Materials Computational Center Travel Award to attend the 7th TDDFT School and Workshop University of Illinois - Urbana-Champaign, IL, USA	2016
LLNL Students Poster Symposium Outstanding Accomplishment Award Lawrence Livermore National Laboratory - Livermore, CA, USA	2015
Eli Lily Scholarship Purdue University - West Lafayette, IN, USA	2014
Young Scientist and Innovator Scholarship of 2011 Administrative Department of Science, Technology, and Innovation of the Colombian Government (Colciencias) and Universidad Icesi - Cali, Colombia	2011

Addendum

Peer-reviewed Articles

Published

- 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
- **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.jpbc.5b11230
Featured in the cover art.
- 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
- 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
- **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
- 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
- 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
- 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



In Press

- 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*, (In press), **2018**. DOI: 10.1021/acs.molpharmaceut.8b00324

In Preparation (Draft available)

- 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. *Manuscript in Preparation*, **2018**.
- **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*, **2018**.
- **Carlos H. Borca**, Brandon W. Bakr, Lori A. Burns, and C. David Sherrill. CrystaLattE: Automated Computation of Benchmark-level Lattice Energy of Molecular Crystals. *Manuscript in Preparation*, **2018**.

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

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.....

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

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 2016) - Philadelphia, PA, USA 8/2016

o *CAM-LDA0: The Reincarnation of the Local Density Approximation*

o *Timescale Separation between Energy Contributions in the Effective Fragment Potential*

o *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 2015) - Boston, MA, USA 8/2015

o *Charge Transfer in the Lithium-Benzene Complex via Density Functional Theory*

o *Developing materials-modeling software for electron dynamics with van der Waals interactions*

o *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.....

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

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 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 <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.....

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 2017 (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 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