# 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 pharmaceutics
- 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-range 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** 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

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|---|---|---|
| Spanish: | Native speaker. | |
| English: | Fluently spoken and written. | *Live and work in the United States since 2012.* |
| Portuguese: | Intermediate proficiency. | |

## Computer Skills

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|---|---|
| Chemistry: | LibEFP/EFPMD, 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.<br>Windows \| 98, XP, Vista, 7, 8, 10. |
| Basic programing: | 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 2018
Carnegie Mellon University - Pittsburgh, PA, USA

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

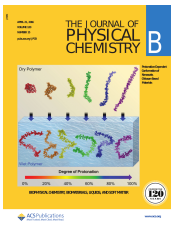
**Eli Lily Scholarship** 2014
Purdue University - West Lafayette, IN, USA

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

# 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.jpcb.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 $\alpha$-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
- 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

### In Press

- 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*, (*In press*), **2018**. DOI: 10.1021/acs.biomac.8b01280

### In Preparation (Draft available)

- **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

**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

**256th National Meeting & Exposition of the American Chemical Society (ACS 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*

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
- *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 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

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 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

**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 2017 (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 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