# Carlos H. Borca | Curriculum Vitæ

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## Summary

A pragmatic theoretical chemist that enjoys engaging problems involving real-life applications and developing original scientific software solutions. Currently, appointed as a postdoctoral fellow in the group of Prof. C. David Sherrill, in the School of Chemistry and Biochemistry at the Georgia Institute of Technology. Postdoctoral research focused on *ab initio* methods for molecular crystals. Graduated with a Ph. D. from the Department of Chemistry at Purdue University, working in the group of Prof. Lyudmila V. Slipchenko. Doctoral research carried out on polarizable molecular dynamics and density functional approximations to approach intermolecular interactions. Summer intern at the Lawrence Livermore National Laboratory during the Computational Chemistry and Materials Science Institute of 2015. Awarded with the Young Scientist and Innovator of 2011 Scholarship by the Government of Colombia. Lecturer of general and physical chemistry laboratories at Universidad Icesi in Cali, Colombia. Honors graduate with a 5-year mayor in Chemistry at Universidad del Valle also in Cali, where consistently ranked top-5-in-class or above.

## Education

**Ph.D. in Chemistry** 8/2012 - 5/2017
Purdue University - Department of Chemistry - West Lafayette, IN, USA

**Applied Management Principles Mini-MBA** 5/2016 - 6/2016
Purdue University - Krannert School of Management - West Lafayette, IN, USA

**Professional (5-Year) Degree in Chemistry** | Honors mention for meritorious research thesis 8/2004 - 11/2009
Universidad del Valle - School of Natural and Exact Sciences - Cali, Colombia

## Experience

### Research Projects

**Development of computational methods for molecular crystals** 8/2017 - Present
Adviser: Prof. C. David Sherrill | Georgia Institute of Technology - Atlanta, GA, USA

**Timescale separation of energy contributions in the effective fragment potential method** 1/2014 - 5/2017
Adviser: Prof. Lyudmila V. Slipchenko | Purdue University - West Lafayette, IN, USA

**Modular implementation of the Tkatchenko-Scheffler model for van der Waals interactions** 6/2015 - 8/2015
Advisers: Dr. Alfredo A. Correa and Dr. Xavier I. Andrade | Lawrence Livermore National Laboratory - Livermore, CA, USA

**Charge-transfer in carbon nanopore models via ground-state density functional theory** 8/2012 - 12/2014
Advisers: Prof. Adam Wasserman and Prof. Lyudmila V. Slipchenko | Purdue University - West Lafayette, IN, USA

**Molecular modeling of water absorbent materials at the nano-scale** 1/2011 - 7/2012
Adviser: Prof. Carlos A. Arango | Universidad Icesi - Cali, Colombia

**Computational study of interactions of single-wall carbon nanotubes/DNA hybrids and small molecules relevant to chemical sensing applications** 8/2007 - 9/2009
Adviser: Prof. Julio C. Arce | Universidad del Valle - Cali, Colombia

### Teaching

**Graduate Teaching Assistant** 8/2012 - 5/2015
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*

**Laboratory Lecturer** 8/2009 - 5/2011
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*

## Honors and Awards

Materials Computational Center Travel Award to attend the 7th TDDFT School and Workshop 9/2016
University of Illinois - Urbana-Champaign, IL, USA

Colombian Students Association at Purdue University (CSAP) Travel Grant Award 8/2015
Purdue University - West Lafayette, IN, USA

**LLNL Students Poster Symposium Outstanding Accomplishment Award** 7/2015
Lawrence Livermore National Laboratory - Livermore, CA, USA

**Eli Lily Scholarship** 6/2014
Purdue University - West Lafayette, IN, USA

**Young Scientist and Innovator Scholarship of 2011** 1/2011
Administrative Department of Science, Technology, and Innovation of the Colombian Government (Colciencias) and Universidad Icesi - Cali, Colombia

**Honors graduation with a mention for meritorious research thesis** 11/2009
Universidad del Valle - Cali, Colombia

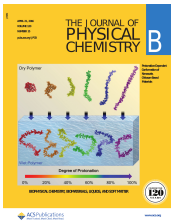
Top-5-in-class Scholarship: six out of eight semesters, including two first places 6/2008
Universidad del Valle - Cali, Colombia

**11$^{th}$ National ICFES Average Score** (Colombian ICFES is analogous to the SAT in the USA) 4/2004
Ministry of Education of the Colombian Government - Bogotá, Colombia

Andrés Bello Departmental Award for the best Biology score in the ICFES 4/2004
Ministry of Education of the Colombian Government - Bogotá, Colombia

## 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

### In Review

- 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. *In review*, **2018**.

### In Preparation

- 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**.
- **Carlos H. Borca**, Alfredo A. Correa, and Xavier I. Andrade. Modular Implementation of Tkatchenko-Scheffler Model for van der Waals Interaction. *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

**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

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

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

### Outreach Programs and Initiatives

Interchange Program 2016 - West Lafayette, IN, USA 7/2016
*Theoretical and Computational Chemistry Science Club*

**Clubes de Ciencia - Colombia 2015 - Puerto Triunfo, Antioquia, Colombia** 10/2015
*Computational Chemistry Science Club Designer and Instructor*

Interchange Program 2015 - Medellín, Antioquia, Colombia 9/2015
*Chemistry and Biology Instructor*

## Professional Affiliations

Member of the American Chemical Society (ACS) 7/2013 - Present

Member of the Colombian Student Association at Purdue University (CSAP) 7/2012 - Present

Member of the Professional Chemists Council of Colombia (CPQ) 2/2010 - Present
*Professional Card No.: PQ-3170*

Jesuit Alumni Association of Cali, Colombia (A.S.I.A. Santiago de Cali) 5/2004 - Present
*Member of the Board (2008-2012)*

## 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. |
| Basic programing: | Python, HTML, C/C++. |
| Others: | Git, Bash, LaTeX, gnuplot, Origin, GIMP, Inkscape, Office, LibreOffice. |

## References

**Prof. C. David Sherrill** | *Postdoctoral Adviser* 8/2016 - Present
Professor - Department of Chemistry - Georgia Institute of Technology
Email: sherrill@gatech.edu | Office Phone: +1 (404) 894-7452

**Prof. Lyudmila V. Slipchenko** | *Doctoral Adviser* 8/2012 - Present
Associate Professor - Department of Chemistry - Purdue University
Email: lslipchenko@purdue.edu | Office Phone: +1 (765) 494-5255

**Prof. Adam Wasserman** | *Committee Member* 8/2012 - 8/2017
Associate Professor - Department of Chemistry - Purdue University
Email: awasser@purdue.edu | Office Phone: +1 (765) 494-2348

**Prof. Lynne S. Taylor** | *Research Collaborator* 8/2014 - 8/2017
Retter Professor of Pharmacy - Department of Industrial and Physical Pharmacy - Purdue University
Email: lstaylor@purdue.edu | Office Phone: +1 (765) 496-6614

## Interests

- Computer repair and upgrade.
- LEGO®.
- Aircraft modeling and simulation.
- Automobile mechanics.