

## Research Focus

Simulation and theory in transport phenomena of complex fluids and soft materials, including the rheology of polymer melts and solutions, liquid crystal polymer systems, polycatenanes, and biopolymers in nanoconfinement, aim to advance our understanding of their structural and dynamic properties, as well as their potential applications

## Education

**Ph.D.**, Department of Chemical Engineering, Universidad de Concepción 2017–2022

Thesis: The Role of an Underlying substrate on confined water in 2D nanoconduits: an atomistic study

Adviser: [Prof. Harvey A. Zambrano](#)

**B.Sc. (Professional qualification)**, Department of Chemical Engineering, Universidad de Concepción 2010–2016

## Professional Experience

**Assistant Professor** ([profile](#)), Department of Chemical Engineering, Universidad de Concepción 2024–Present

**Post Doctoral Scholar** ([Hall Research Group](#)), William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University 2022–2023

Adviser: [Prof. Lisa M. Hall](#).

## Honors & Awards

Outstanding Post-Doctoral Fellow (Chemical Engineering). William G. Lowrie Department of Chemical and Biomolecular Engineering. The Ohio State University. *American Institute of Chemists Foundation* 2023

[Society of Rheology Postdoc Poster Award runner up](#) with "Polymer Rheology Predictions from First Principles using the Slip Link Model" 2022

Doctor of Engineering Sciences (Chemical Engineering) degree obtained with highest distinction. 2022

Chemical Engineering degree obtained with highest distinction. 2016

## Publications

### Published in peer-reviewed journals

- [1] Reentanglement Dynamics in Polymer Melts Can Be Explained by Fast Dangling End Retraction without Resorting to Nonuniversality  
Andrés Córdoba, **Diego Becerra**, Jay D Schieber  
*ACS Macro Letters* 14.3 (2025), pp. 385–390, ACS Publications  
DOI: <https://doi.org/10.1021/acsmacrolett.4c00809>
- [2] Effect of charge inversion on the electrokinetic transport of nanoconfined multivalent ionic solutions  
Andrés Rojano, **Diego Becerra**, Jens H Walther, Shaurya Prakash, Harvey A Zambrano  
*Physics of Fluids* 36.10 (2024), p. 102025, AIP Publishing  
DOI: <https://doi.org/10.1063/5.0227719>
- [3] Role of Underlying Substrates on the Interfacial Thermal Transport in Supported Graphene Nanochannels: Implications of Thermal Translucency  
**Diego Becerra**, Jens H. Walther, Harvey A. Zambrano  
*Nano Letters* 24.39 (2024), pp. 12054–12061, ACS Publications (**Featured in Front Cover**)  
DOI: <https://doi.org/10.1021/acs.nanolett.4c02106>
- [4] Single-molecule analysis of solvent-responsive mechanically interlocked ring polymers and the effects of nanoconfinement from coarse-grained simulations

**Diego Becerra**, Alexander R. Klotz, Lisa M. Hall  
*The Journal of Chemical Physics* 160.11 (2024), p. 114906, AIP Publishing  
DOI: <https://doi.org/10.1063/5.0191295>

- [5] Conformational variability of intrinsically isotropic polymers with varying stiffness immersed in nematogenic solvents  
**Diego Becerra**, Pranav R. Jois, Lisa M. Hall  
*Polymer* 295 (2024), p. 126774, Elsevier  
DOI: <https://doi.org/10.1016/j.polymer.2024.126774>
- [6] Impact of Molecular-level Structural Disruption on Relaxation Dynamics of Polymers with End-on and Side-on Liquid Crystal Moieties  
**Diego Becerra**, Yang Xu, Xiaoguang Wang, Lisa M. Hall  
*ACS Nano* 17.24 (2023), pp. 24790–24801, ACS Publications  
DOI: <https://doi.org/10.1021/acsnano.3c05354>
- [7] Water flow in a polymeric nanoslit channel with graphene and hexagonal boron nitride wall coatings: An atomistic study  
**Diego Becerra**, Andrés Córdoba, Jens H. Walther, Harvey A. Zambrano  
*Physics of Fluids* 35.10 (2023), p. 102009, AIP Publishing  
DOI: <https://doi.org/10.1063/5.0165657>
- [8] Coarse-grained modeling of polymers with end-on and side-on liquid crystal moieties: Effect of architecture  
**Diego Becerra**, Pranav R. Jois, Lisa M. Hall  
*The Journal of Chemical Physics* 158.22 (2023), p. 224901, AIP Publishing  
DOI: <https://doi.org/10.1063/5.0152817>
- [9] Examination of Nonuniversalities in Entangled Polymer Melts during the Start-Up of Steady Shear Flow  
**Diego Becerra**, Andrés Córdoba, Jay D. Schieber  
*Macromolecules* 54.17 (2021), pp. 8033–8042, ACS Publications (**Featured in Front Cover**)  
DOI: <https://doi.org/10.1021/acs.macromol.1c00156>
- [10] Polymer rheology predictions from first principles using the slip-link model  
**Diego Becerra**, Andrés Córdoba, Maria Katzarova, Marat Andreev, David C. Venerus, Jay D. Schieber  
*Journal of Rheology* 64.5 (2020), pp. 1035–1043, The Society of Rheology  
DOI: <https://doi.org/10.1122/8.0000040>
- [11] Water flow enhancement in amorphous silica nanochannels coated with monolayer graphene  
Enrique Wagemann, **Diego Becerra**, Jens H. Walther, Harvey A. Zambrano  
*MRS Communications* 10.3 (2020), pp. 428–433, Cambridge University Press  
DOI: <https://doi.org/10.1557/mrc.2020.53>

## Contributed Talks

Presentations are listed in reverse chronological order, and the presenting author is in bold.

- [1] Relation between Structural Disruption and Memory Effects in Side-Chain Liquid Crystal Elastomers Fracture of Soft Polymeric Materials  
**Diego Becerra**, Gabriel Schiappacasse, and José M. Garrido, APS Global Physics Summit; Anaheim, United States; March 20, 2025
- [2] Probing the relationship between wall misalignment and water transport properties in sub-nm hexagonal boron nitride slit channels  
**Enrique Wagemann**, Elton Oyarzúa, Diego Becerra, and Harvey Zambrano, 77th Annual Meeting of the Division of Fluid Dynamics; Salt Lake City, United States; November 26, 2024
- [3] Coarse-grained simulations of side chain liquid crystal polymers with different types of attachments  
Diego Becerra and **Lisa M. Hall**, AIChE Annual Meeting; Orlando, United States; November 6, 2023
- [4] Effect of the mesogenic type of attachment and composition on the structural and viscoelastic behavior of side-chain liquid crystal polymer systems  
**Diego Becerra** and Lisa M. Hall, APS March Meeting; Las Vegas, United States; March 7, 2023
- [5] Rheology of linear polymer melts with end-on and side-on liquid crystal moieties in different phases: Effects of composition and thermodynamical state on relaxation dynamics  
**Diego Becerra** and Lisa M. Hall, Society of Rheology 93rd Annual Meeting; Chicago, United States; October 11, 2022
- [6] Examination of non-universalities in entangled polymer melts and solutions during the startup of steady

shear flow

Diego Becerra, **Andrés Córdoba**, and Jay D. Schieber, Society of Rheology 93rd Annual Meeting; Chicago, United States; October 10, 2022

- [7] **A Coarse-Grained Model for Side-Chain Liquid Crystalline Linear Polymers**  
**Diego Becerra** and Lisa M. Hall, 52nd Midwest Theoretical Chemistry Conference; Columbus, United States; June 3, 2022
- [8] **Examination of non-universalities in entangled polymer melts and solutions during the startup of steady shear flow**  
**Jay D. Schieber**, Diego Becerra, and Andrés Córdoba, APS March Meeting; Chicago, United States; March 17, 2022
- [9] **Predicting Several Seconds of the Relaxation Dynamics of an Entangled Polymer Melt from a Few Nanoseconds of Atomistic Molecular Dynamics**  
**Diego Becerra**, Andrés Córdoba, and Jay D. Schieber, APS March Meeting; Chicago, United States; March 15, 2022
- [10] **Effect of Interfacial Thermal Transport on Water Flow in Graphene Nanochannels**  
**Diego Becerra**, Jens H. Walther, and Harvey A. Zambrano, APS March Meeting (virtual); United States; March 16, 2021
- [11] **Effect of Underlying Substrate on Interfacial Heat Transfer in Graphene Channels**  
**Diego Becerra**, Jens H. Walther, and Harvey A. Zambrano, 73rd Annual Meeting of the American Physical Society Division of Fluid Dynamics (virtual); Chicago, United States; November 23, 2020
- [12] **Effect of Charge Inversion on Electroosmotic Transport in Nanochannels**  
**Andrés Rojano**, Diego Becerra, Jens H. Walther, and Harvey A. Zambrano, 73rd Annual Meeting of the American Physical Society Division of Fluid Dynamics (virtual); Chicago, United States; November 23, 2020
- [13] **Hydrodynamics in a Polymeric Nanoslit Pore with Graphene Wall Coating: An Atomistic Study**  
**Diego Becerra**, Andrés Córdoba, Jens H. Walther, and Harvey A. Zambrano, MRS Fall Meeting & Exhibit; Boston, United States; December 6, 2019
- [14] **Hydrodynamics in a Polymeric Nanoslit Pore with Graphene and Hexagonal Boron Nitride Wall Coatings: An Atomistic Study**  
**Diego Becerra**, Andrés Córdoba, Jens H. Walther, and Harvey A. Zambrano, 72nd Annual Meeting of the American Physical Society Division of Fluid Dynamics; Seattle, United States; November 26, 2019
- [15] **Molecular Dynamics study of the hydrodynamics in a polymeric slit channel with graphitic wall coating**  
**Diego Becerra**, Andrés Córdoba, and Harvey A. Zambrano, 71st Annual Meeting of the American Physical Society Division of Fluid Dynamics; Atlanta, United States; November 19, 2018

## Contributed Posters

Posters are listed in reverse chronological order and the presenting author is in bold.

- [1] **Polymer rheology predictions from first principles using the slip-link model**  
**Diego Becerra**, Andrés Córdoba, Maria Katzarova, Marat Andreev, David C. Venerus, and Jay D. Schieber, Society of Rheology 93rd Annual Meeting; United States; October 12, 2022
- [2] **The Importance of Non-Universalities in Entangled Polymer Melts During the Startup of Steady Shear Flow**  
**Diego Becerra**, Andrés Córdoba, and Jay D. Schieber, APS March Meeting (virtual); United States; March 17, 2021

## Teaching Experience

**Instructor**, FI 540722, FI 406203, FI 4219041, *Fenómenos de Transporte*, Graduate course, Universidad de Concepción  
2025-I

**Instructor**, FI 540265, *Mecánica de Fluidos*, Undergraduate course, Universidad de Concepción  
2024-II

**Instructor**, FI 540353, *Taller de Integración II*, Undergraduate course, Universidad de Concepción  
2024-II

**Instructor**, FI 540264, *Termodinámica*, Undergraduate course, Universidad de Concepción  
2024-I, 2025-I

**Instructor**, FI 540261, *Laboratorio de Procesos Químicos*, Undergraduate course, Universidad de Concepción  
2024-I

**Teaching (cover lessons)**, CHBE 3508, *Thermodynamics: Lectures on the Thermodynamics of Multicomponent Mixtures*, Undergraduate course, The Ohio State University  
Spring 2023

**Teaching (cover lessons)**, CHBE 8808, *Advanced Thermodynamics: Lectures on Statistical Mechanics*, Graduate course, The Ohio State University  
Fall 2022

## Thesis Supervision and Committee Work

**Undergraduate Thesis Committee Member**, Paula Soto Montecinos, "Producción y caracterización de películas de nanocelulosa sulfatada aditivadas con cationes metálicos" 2025  
Ingeniería Civil Química, Universidad de Concepción

**Undergraduate Thesis Committee Member**, José Campos Castro, "Análisis del rendimiento de un sistema de electrodiálisis con membrana catiónica para la recuperación de hidróxido de litio a partir de cloruro de litio" 2025  
Ingeniería Civil Química, Universidad de Concepción

**Undergraduate Thesis Supervisor**, Maximiliano Sepúlveda Irrarrázabal, "CFD-Based Studies and Model Development for Top-Blown Rotary Converters (TBRC)" 2025  
Ingeniería Civil Química, Universidad de Concepción

**Master's Thesis Committee Member**, Pablo Felipe Caniu Villablanca, "Análisis y validación de un modelo molecular de grafeno utilizando potencial Tersoff polarizable mediante simulaciones de dinámica molecular" 2024  
Ingeniería Civil Mecánica, Universidad de Concepción

**Undergraduate Thesis Committee Member**, Manuel Astroza Olivella, "Desarrollo de estructuras metálicas porosas, para aplicación en soportes de celdas de combustible de óxido sólido" 2024  
Ingeniería Civil de Materiales, Universidad de Concepción

**Undergraduate Thesis Committee Member**, Johairo Núñez Aguayo, "Estudio de la interacción de nanofibra de celulosa con nanopartículas de lignina" 2024  
Ingeniería Civil Química, Universidad de Concepción

## Mentoring Experience (Advisees)

1 current Master's program undergraduate student: Gabriel Schiappacasse (started 2025-I, Universidad de Concepción)

2 former undergraduate researchers: Fesume Hailu (fall 2022, The Ohio State University; next position at JP Morgan Chase & Co.); Pranav Jois (summer 2022-fall 2023, The Ohio State University; next position at College of Literature, Science, and the Arts, University of Michigan as Ph.D. student)

1 former high school research students: Alasdair DeLong (summer 2023, The Ohio State University)

## Participation in Research Projects

- [1] Relation Between Structural Disruption And Memory Effects In Side-chain Liquid Crystal Elastomers: A Molecular Modeling Approach. FONDECYT  
Role: **Principal Investigator**
- [2] Processing and Properties of Polymer-Grafted Nanoparticle Monolayers. FA9550-23-1-0288. Air Force Office of Scientific Research, United States, 2023–2026.  
Role: **Postdoctoral Scholar and Collaborator**
- [3] Modeling Polymers with End-on and Side-on Liquid Crystal Moieties: Effects of Sequence on Phase Behavior and Thermomechanical Response. New Directions (PRF 62346-ND7). American Chemical Society Petroleum Research Fund; United States, 2022–2023.  
Role: **Postdoctoral Scholar**
- [4] Biomimetic design of soft condensed materials: A molecular modeling approach. FONDECYT Iniciación

11170056. ANID; Chile, 2018–2021.

Role: **Technical staff**

## Academic and University Service

### Reviewer for Journal Articles

*Computational Materials Science*

*Soft Matter*

*Physics of Fluids*

*The Journal of Chemical Physics*

*The Journal of Physical Chemistry B*

**Judge for “12th Annual Graduate Research Symposium (GRS)”, The Ohio State University**

2023

**Chairman, session on “Structure and Dynamics of Ion-Containing Polymers II”**

2022

APS March Meeting, Chicago, United States

## Event Organization and Outreach

**Seminar Series of Soft Matter**, The Ohio State University.

2023

Role: Organization of an internal seminar series for graduate students, postdocs, and professors in Polymer and Soft Matter-focused groups. The Seminars involve scientists from 4 Departments: Chemical and Biomolecular Engineering, Chemistry and Biochemistry, Mechanical Engineering and Food Science and Technology, as well as external invitees.

**Breakfast of Science Champion**, The Ohio State University.

2023

Role: Organization an update of outreach activities of Hall Research Group, in particular, an interactive simulation setup for pure polymers that has been successful in engaging both K-12 students and the general public in understanding the molecular basis of material properties. for better use with K-12 participants.