LORENA ALZATE-VARGAS

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EDUCATION

PhD in Materials Science & Engineering Aug. 2014 - Dec. 2019
Purdue University, West Lafayette, IN
Dissertation: Structural and Dynamical Properties of Organic and Polymeric Systems using Molecular Dynamics Simulations

BSc Engineering Physics Jan. 2010 - Jun. 2014
Universidad EAFIT, Medellín, Colombia

RESEARCH EXPERIENCE

Postdoctoral Research Associate Jan. 2020 - Present
Oak Rigde National Laboratory, Oak Ridge, TN
PI: Dr. Jean-Luc Fattebert & Dr. Sergiy Kalnaus

- Develop a simulation protocol to study at the atomistic level the anode solid electrolyte interface (SEI) on Li ion batteries, including a methodology to model chemical reactions using classical molecular dynamics.
- Study the temporal evolution of the SEI and determine the influence of different reactions on its composition.

Graduate Research Assistant Aug. 2014 - Dec. 2019
Purdue University, West Lafayette, IN
Advisor: Dr. Alejandro Strachan

- Quantified uncertainties in predicted properties of polymeric materials using molecular dynamics simulations and the influence of input variables.
- Studied amorphization in pharmaceutical compounds using molecular dynamics as part of a multiscale modeling framework. Prediction of structural properties.
- Utilized molecular dynamics and cluster analysis to study the nature of the glass transition in polymers and the finite size effects on conformational dynamics and relaxation process.
- Cyber-enabling molecular modeling tools for polymer simulations.

Undergraduate Research Intern Jul. 2013 - Jan. 2014
Purdue University, West Lafayette, IN
Advisor: Dr. Alejandro Strachan

- Developed and implemented a Python algorithm to measure torsional angles and detect conformational transitions.

Undergraduate Research Assistant Jan. 2012 - May. 2013
Universidad EAFIT, Medellín, Colombia
Advisors: Dr. Jorge D. Caro & Mario E. Vélez

- Utilized ab-initio simulations to study structural, electrical and topological properties of CrN compounds obtained from genetic algorithms to determine their possible application as functional coatings.

TOOLS AND SKILLS

Programming	Python, C++
Ab-initio tools	Quantum Espresso, SeqQuest, Crystal, CP2K, Q-Chem
Molecular dynamics	LAMMPS
Other	Solid Works

TEACHING EXPERIENCE

Atomistic Materials Science MSE 237 Spring 2015
Purdue University, West Lafayette, IN
Supervisor: Alejandro Strachan

- Held office hours regularly to answer questions about materials covered in class and in preparation for exams.
- Responsible for assessing students' performance in assignments and exams.

Numerical Methods and CAD Software Fall 2012
Universidad EAFIT, Medellín, Colombia
Supervisor: Mauricio Arroyave

- Helped students with understanding numerical methods and their implementation in Python and MATLAB
- Gave tutorials in computer-aided design used for second year engineering projects.

STUDENT MENTORING

Research Undergraduate Program Summer 2017
LAMMPS data file generator for molecular simulations
Student: Carlos Patiño

Research Undergraduate Program Summer 2015
Thermal properties of polymers using molecular dynamics
Student: Daniel Glass

SCIENTIFIC SOFTWARE

[1] Patiño, Carlos M., **Alzate-Vargas, Lorena**, Li, Chunyu, Haley, Benjamin and Strachan, Alejandro. LAMMPS Data File Generator (2017) https://nanohub.org/resources/struc2lammpsdf

[2] Haley, Benjamin, **Alzate-Vargas, Lorena**, Hunt, Martin and Strachan, Alejandro. Glass Transition Temperature Notebook (2017) https://nanohub.org/resources/tgnb

PUBLICATIONS

[1] **Alzate-Vargas, Lorena**, Onofrio, Nicolas, and Strachan, Alejandro. "Universality in Spatio-Temporal High-Mobility Domains Across the Glass Transition from Bulk Polymers to Single Chains". In: *Macromolecules* 53.21 (2020), pp. 9375–9385. DOI: 10.1021/acs.macromol.0c00853.

[2] Reeve, Samuel. T., Guzman, David. M., **Alzate-Vargas, Lorena**, Haley, Benjamin, Liao, Peilin, and Strachan, Alejandro. "Online Simulation Powered Learning Modules for Materials Science". In: *MRS Advances* 4.50 (2019), pp. 2727–2742. DOI: 10.1557/adv.2019.287.

[3] Zeng, Yifei, **Alzate-Vargas, Lorena**, Li, Chunyu, Graves, Rachel, Brum, Jeff, Strachan, Alejandro, and Koslowski, Marisol. "Mechanically Induced Amorphization of Small Molecule Organic Crystals". In: *Modelling Simul. Mater. Sci. Eng* 27 (2019), p. 074005. DOI: 10.1088/1361-651x/ab234a.

[4] **Alzate-Vargas, Lorena**, Fortunato, Michael E, Haley, Benjamin, Li, Chunyu, Colina, Coray M, and Strachan, Alejandro. "Uncertainties in the Predictions of Thermo-Physical Properties of Thermoplastic Polymers via Molecular Dynamics". In: *Modelling Simul. Mater. Sci. Eng* 26.6 (2018), p. 065007. DOI: 10.1002/pssa.201700576.

[5] Marín-Suárez, Marco, **Alzate-Vargas, Leidy L**, David, Jorge, Arroyave-Franco, Mauricio, and Vélez, Mario E. "Electronic and Topological Analysis for New phases of Chromium Nitride". In: *Phys. Status Solidi A* 215.1 (2018), p. 1700576. DOI: 10.1002/pssa.201700576.

[6] **Alzate-Vargas, Lorena**, Li, Chunyu, Haley, Benjamin, Fortunato, Michael, Colina, Coray, and Strachan, Alejandro. "Uncertainties of Parameters to Predictions of Polymer Properties by Molecular Simulations". In: *American Society for Composites*. DEStech Publications, Inc., 2017.