

# ARSENI PANTELEEV

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## EDUCATION

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### University of Notre Dame

Bachelor of Science in Chemical Engineering  
Minor in Chinese Studies

August 2016 - May 2020

GPA: 3.48

GPA: 3.81

### UC Irvine

MS/PhD in Chemical Engineering

September 2020 - June 2026

GPA: 3.9

## RESEARCH EXPERIENCE

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### In-Situ TEM Determination of Solid-State Diffusion Kinetics for the Aluminum-Nickel System

Spring 2018, under the supervision of Prof. A. S. Mukasyan

Implemented the experimental model in the simulation software Comsol Multiphysics, through which our research group validated the new method of determination of solid-state diffusion kinetics for the Aluminum-Nickel system.

### Replica-Exchange Simulations of the Crystal-Smectic-A Transition in Ionic Liquid Crystals

Summer 2018 - Present, under the supervision of J. K. Whitmer, joined Whitmer Research Group the same year

Performed Replica-Exchange simulations on the system of 512 pairs of alkyl-imidazolium nitrate salts,  $[C_nMIm][NO_3]$ , and investigated the trends in melting points by changing the carbon chain length. As a result, identified the transition temperatures for  $C_{10}MIm$  and  $C_{18}MIm$ . The calculations later were included in the paper, and the data will later become a part of the application for DOE ECRP \$750k grant, "Computational Studies of Ionic Liquid Crystals".

### Physical mechanisms of Hofmeister effects

Summer 2018 - Present, under the supervision of J. K. Whitmer and as a part of Whitmer Research Group

Investigated the physical mechanisms of Hofmeister effects by modeling a system of 512 Stockmayer fluid particles and an ion in molecular simulation package LAMMPS. By changing the dipole moment of the ion (with the dipole moment kept constant on the solvent particles), identified a correlation between the dipole of the ion and its affinity to adsorb to the surface of the fluid. The results will be submitted as a paper targeted for the *Journal of Chemical Physics*.

### Determination of elastic constants of LJ crystal using SSAGES

Summer 2019 - Present, under the supervision of J. K. Whitmer and as a part of Whitmer Research Group

Built a system of 864 particles in LAMMPS, and using SSAGES (Software Suite for Advanced General Ensemble Simulations) analyzed different elastic modes of an LJ crystal. Wrote several add-ons for the basic version of SSAGES (C++), extensively used Python and GDB for debugging purposes. We're aiming to prove that different elastic modes can be sampled by fixing the edge of the crystal using Umbrella sampling and by using ABF on the plane in the center of the crystal. Results pending.

## TECHNICAL STRENGTHS

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### Analysis

MATLAB, Python, GDB

### Software & Tools

MS Office, Latex, LabVIEW, Unix, GROMACS, LAMMPS, COMSOL, C++ (basic)

### Languages

Russian, English, Mandarin

## NCAA ATHLETICS

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### University of Notre Dame DIV1 Fencing team

- 2017, 2018 NCAA Team champion, 2017, 2019 ACC Team champion
- 2019 Midwest Regional Champion

## LEADERSHIP

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### Rosenthal Leadership Academy

Notre Dame, IN

Fall 2017 - Spring 2018

- Nominated on behalf of peers, coaches, and support staff to represent the program in monthly meetings, retreats, and workshops

## CONTRIBUTED TALKS AND POSTERS

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### APS March Meeting 2019

- Modeling the Properties of Liquid Crystal Electrolytes with Replica Exchange Molecular Dynamics. J. K. Whitmer, M. J. Quevillon, A. Pantelev.

## **AWARDS AND HONORS**

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- The Vincent P. Slatt Fellowship for Undergraduate Research in Energy Systems and Processes, University of Notre Dame, 2018
- Chemical Engineering Research Award, University of Notre Dame, 2020