SLATT UNDERGRADUATE RESEARCH FELLOWSHIP
FINAL REPORT

SCHOLAR NAME:	Jiaqi Lu
FACULTY ADVISOR:	Yamil J. Colón
PROJECT PERIOD:	Spring/Fall 2022
PROJECT TITLE:	Transfer learning from density to refractive index and to density across temperatures for ionic liquids
CONNECTION TO ONE OR MORE ENERGY-RELATED RESEARCH AREAS (CHECK ALL THAT APPLY):	**(x) Energy Conversion and Efficiency** **( ) Sustainable and Secure Nuclear** **( ) Smart Storage and Distribution** **( ) Transformation Solar** **( ) Sustainable Bio/Fossil Fuels** **( ) Transformative Wind**

MAJOR GOALS AND ACCOMPLISHMENTS

Summarize your research goals and provide a brief statement of your accomplishments (no more than 1-2 sentences). Indicate whether you were able to accomplish your goals by estimating the percentage completed for each one. Use the next page for your written report.

RESEARCH GOALS	ACTUAL PERFORMANCE AND ACCOMPLISHMENTS	% OF GOAL COMPLETED
Use machine learning to predict thermodynamic properties of ionic liquids	Built dense neural networks that is able to predict ionic liquid density at 298-299 K and predict ionic liquid refractive index at various temperatures with high accuracy	100%
Demonstrate the transferability of predicting ionic liquids thermodynamics properties at atmospheric pressure	Applied transfer learning to predicting ionic liquid density at various temperatures and ionic liquid refractive index based on limited data, with apparent improvement in accuracy in comparison to direct learning	100%
Offer possible explanation to validate the applicability of transfer learning in each case	Performed feature importance analysis to validate the transferability in each case	100%

RESEARCH OUTPUT

Please provide any output that may have resulted from your research project. You may leave any and all categories blank or check with your faculty advisor if you are unsure how to respond.

CATEGORY	INFORMATION
EXTERNAL PROPOSALS SUBMITTED	(Sponsor, Project Title, PIs, Submission Date, Proposal Amount)
EXTERNAL AWARDS RECEIVED	(Sponsor, Project Title, PIs, Award Date, Award Amount)
JOURNAL ARTICLES IN PROCESS OR PUBLISHED	Transfer learning from density to refractive index and to density across temperatures for ionic liquids, in process
BOOKS AND CHAPTERS RELATED TO YOUR RESEARCH	(Book Title, Chapter Title, Authors, Submission Date, Publication Date, Volume #, Page #s)
PUBLIC PRESENTATIONS YOU MADE ABOUT YOUR RESEARCH	(Event, Presentation Title, Presentation Date, Location)
AWARDS OR RECOGNITIONS YOU RECEIVED FOR YOUR RESEARCH PROJECT	(Purpose, Title, Date Received)
INTERNAL COLLABORATIONS FOSTERED	(Name, Organization, Purpose of Affiliation, and Frequency of Interactions)
EXTERNAL COLLABORATIONS FOSTERED	(Name, Organization, Purpose of Affiliation, and Frequency of Interactions)
WEBSITE(S) FEATURING RESEARCH PROJECT	(URL)
OTHER PRODUCTS AND SERVICES (e.g., media reports, databases, software, models, curricula, instruments, education programs, outreach for ND Energy and other groups)	(Please describe each item in detail)

RESEARCH EXPERIENCE

Please let us know what you thought of your research experience: Did this experience meet your expectations? Were lab personnel helpful and responsive to your needs? What else could have been done to improve your experience or achieve additional results?

The original goal of this research is to apply transfer learning for ionic liquids from density to viscosity, but later I discovered that while the attempt to proceed in the original direction failed to give satisfactory results, I was able to apply transfer learning from density to refractive index, and furthermore, from density at one temperature to density at another temperature. Since my overarching goal is to see if transfer learning is applicable in predicting thermodynamics properties of ionic liquids, this research finding and later progress has met my expectation. This project is advised by Professor Yamil J. Colón and Ph.D. student Fernando J. Carmona Esteva. I would like to thank them for being very helpful and responsive throughout the process. To achieve additional results, we can try new descriptors that gives more accurate prediction of new thermodynamic properties that I previously was not able to achieve.

FINAL WRITTEN REPORT

(Please use the space below to describe your research project and objectives, any findings and results you can share, and graphs, charts, and other visuals to help us understand what you achieved as a result of this research experience.)

In this work, we built dense neural networks (DNNs) to show the transferability of predicting ionic liquids thermodynamics properties at approximately 101 pKa: (1) from density at room temperature to density at three other temperatures and (2) from density to refractive index at various temperatures. By transferring DNN weights trained from predicting density at 298 K to predicting density at three other temperatures, the average accuracies on target tasks trained with 10 data points improved, from 10%, 13%, and 11% MAPE (direct) to 3%, 3%, and 4% MAPE (transfer). By transferring knowledge gained from predicting density to predicting refractive index, the average accuracy on target task trained with ~40 data points improved, from 4% MAPE (direct) to 1% MAPE (transfer). In both scenarios, transfer learning works in the majority of the cases.

This research yields a manuscript in write-up, more details will be shared once preprint is available.