SPS Chapter Research Award Proposal

Project Proposal Title	Ionic Conductivity of the Lithium Clustering Effect
Name of School	Coe College
SPS Chapter Number	1255
Total Amount Requested	$2,000.00

Abstract

The Coe College SPS Chapter will investigate the lithium clustering effect on silicate and borate glasses for better understanding the ionic diffusion due to electric fields and ionic conductivity. SPS members will learn how to prepare glass samples, conduct electrical impedance spectroscopy measurements, and witness the novel lithium clustering effect.

Proposal Statement

Overview of Proposed Project

This research will expand our understanding of glass properties, expose us to novel conductivity testing methods and analysis, as well as strengthen our relationship with the Glass and Optical Research Group, part of the Materials Science and Engineering Department, at Iowa State University (ISU). We will study chemical glass formations and gain hands-on research experience with novel testing equipment in materials science development. This includes glass characterization, such as density measurements, differential calorimetry scanning, impedance spectroscopy at low frequencies, X-ray diffraction and others.

Physicists have documented ion conductivity plateaus with lithium glass systems when ion counts continue to increase. Generally, the more ions available to pass charge would result in a greater conductivity; however, systems containing high amounts of lithium do not follow this trend. Currently, there is not an explanation for this phenomenon, but molecular dynamics (MD) simulations lead us to believe lithium ions are clustering when presented in high enough concentrations, inhibiting the ions from passing charges and resulting in a constant ionic conductivity. Our goal is to examine this hypothesis by preparing x Li_2O (1-x) B_2O_3 and x Li_2O (1-x) SiO_2 glasses, with x= 0.2, 0.3, 0.4, 0.5, and 0.6 to identify the region of the ionic conductivity plateau.

By researching the ionic conductivity of glasses with high lithium concentration, younger SPS members will be able to learn proper laboratory techniques and procedures from our well-trained SPS researchers which fosters mentor/mentee relationships. SPS members will also be able to participate in the entire research process from balancing chemical equations and mixing samples to cooling glass in a roller quencher and performing analysis at another institution. Our collaboration with ISU will be the foundation of new partnerships for the Coe College Society of Physics Students. The project advisor, Dr. Caio Bragatto, will give a talk at ISU and Coe College on his work on conductive properties in glass systems. Likewise, we will host Dr. Steve W. Martin, a well-known glass scientist at ISU, at Coe College for a day to present his work and give a seminar on glass conductivity for all Coe College SPS members, and his research group.

Background for Proposed Project

Glass conductivity depends on the number of available charge carriers and their speed [1]. For ionic materials, the charge carrier is almost always an alkali (elements from the Group 1A of the periodic table) or monovalent metals, due their higher conductivity when compared to other ions [2]. This leads scientists to expect glasses with higher alkali ion concentrations to have greater ionic conductivity since more charge carriers should be available to diffuse. However, this is not the case for the ionic conductivity of glasses with a high concentration of lithium [3,4]. The literature often interprets this maximum ionic conductivity effect as experimental error from phase separation. Recent works attribute this phenomenon to a change in the glass structure due the high concentration of glass modifiers in the borate system [3]. Unfortunately, this would not explain the behavior observed in lithium silicate glasses.

Classical molecular dynamics (MD) simulations have shown lithium ions exhibiting a clustering effect in glass matrices which trap additional lithium ions [5]. This might explain the plateau found for the ionic conductivity at higher concentrations. Due the formation of the clusters, less lithium ions are available to move than expected. Since there is still no consensus in the literature to what causes this change in the slope of ionic conductivity versus composition, more studies about the subject are necessary. For that, we want to prepare homogeneous glasses with high lithium concentration and study their ionic conductivity. The preparation of these glass samples is only possible due to the fast roller-quenching technique available at Coe College.

Expected Results

The glass samples prepared, with an extremely high cooling rate, are expected to be homogeneous and with no phase separation. By eliminating this possible experimental error, results found can be directly related to the clustering effect. If the conductivity shows the plateau, even though the samples prepared are homogoeneous and have no phase separation, we can attribute the outcome to the clustering effect. If the results show no plateau, then the cluster has no significant effect on the diffusion of the Li ions through the glass matrix. Either result will contribute to the discussion and importance of the formation of the Li cluster to the glass properties, creating a more definite understanding of lithium containing glass systems.

Description of Proposed Research - Methods, Design, and Procedures

The glasses will be prepared by the mixing and melting of adequate amount of lithium carbonate and boric acid or silica powder for each sample composition. After mixing, the powders will be melted for 30 min to 1 hour at temperatures 200 ^{o}C above the liquidus temperature. The liquidus temperature depends on the glass composition, but we know from the literature and previous experience that they range from 700 ^{o}C to 1200 ^{o}C. Normally glasses are prepared by splash-quenching techniques, i.e. the glass is cooled by pouring the melt on top of a metalic block and pressing it with another metalic piece, to cool it down fast enough and avoid crystalization. For glasses containing a high concentration of lithium, this method is not enough to avoid this phase separation, therefore we need to use some technique with an even higher cooling rate. The easiest and more guaranteed way to obtain homogeneous glasses is by roller-quenching the melt. The roller-quencher we will be using for this work was fabricated by the Physics Department at Coe College.

These glass samples will then be tested and characterized – by X-ray diffraction (XRD) to test homogeneity and amorphous structure, by differential scanning callorimetry (DSC) to determine important first and second order changes in the specific heat of the samples, which can be related respectively to crystallization temperatures (T_c) and glass transition temperature range (T_g), by scanning electronic microscopy (SEM) to better understand possible phase separations and crystallization of the samples, and finally by electrical impedance spectroscopy (EIS) to characterize the electrical properties of each phase present in the glass samples.

Plan for Carrying Out Proposed Project

- Personnel
  - Project Manager: Anne Ruckman – Overseeing research deadlines and leading experimental development as outlined in the Project Timeline to ensure project success
  - Lead Glass Researcher: Martha Jesuit – Creating glass samples
  - Lead Computational Researcher: Wataru Takeda – Simulating glass compositions
  - Computational Researcher: Rebecca Welch – Conducting MD simulations of glasses
  - Project Advisor: Dr. Caio Bragatto – Instructing SPS researchers and facilitating experimentation and analysis
  - Faculty Supporters: Dr. Steve Feller, Dr. Mario Affatigato - Supporting SPS members and clarifying techniques for first-time researchers
  - SPS member participation:
    - 3-5 SPS members will conduct research as mentees of the lead researchers
    - 10-15 SPS members will travel to ISU to analyze our samples
    - All SPS members and non-members are encouraged to attend Dr. Martin's lecture
    - All SPS members and non-members are encouraged to attend Dr. Bragatto's talk
- Expertise
  - There are several SPS members who will lead our research proposal.

- Anne Ruckman is the Outreach Coordinator for Coe College Women in STEM and Historian of the Coe College SPS chapter. Anne successfully oversaw the SPS Future Faces of Physics Award in 2017-2018, and has experience managing local grants from our institution. She also brings extensive research experience as fellow from the U.S. Department of Energy National Energy Technology Lab.
- MaryJane Been is President of the Coe College SPS Chapter and Vice President of Coe College Women in STEM. Her experience as a senior physics researcher, and chapter leader will reinforce our project goals and objectives.
- Martha Jesuit is the Secretary of the Coe College SPS chapter, and Vice President of the Coe College Math Club. She has studied borate glass systems, and produced samples for two years. Her glass making techniques will lead the investigation of the novel clustering effect.
- Dr. Steve Feller & Dr. Mario Affatigato have extensive experience in glass studies

- Research space
  - Coe College Physics Department will contribute lab space and use of glass formation resources on campus in Peterson Hall. All tests except for impedance spectroscopy will be conducted at Coe College.
  - Iowa State University's Material Science and Research Department will contribute space and time on their impedance spectrometer for advanced conductivity testing.

Project Timeline

Dates	Objectives	Officers Involved
January 14-25, 2019	Purchase required chemicals and materials, Introduce mentor/mentee SPS members	Anne Ruckman
January 14-31, 2019	Dr. Caio Bragatto's lecture on ionic conductivity at Coe College	Anne Ruckman
January 25-March 15, 2019	Create glass samples, Run MD simulations for glass ratios	Martha Jesuit, Wataru Takeda, Anne Ruckman
February 15-May 30, 2019	Dr. Steve Martin gives his seminar on electrical properties at Coe College	Anne Ruckman
March 1-April 30, 2019	Dr. Caio Bragatto gives his seminar on glass conductivity at Iowa State University	Anne Ruckman
March 15-May 30, 2019	SPS members test glasses at Coe College and Iowa State University	Anne Ruckman, Martha Jesuit, Wataru Takeda
May 31, 2019	Compile interim report	Anne Ruckman
June 1-November 15, 2019	SPS members analyze glass conductivity and submit research paper	Anne Ruckman, Martha Jesuit, Wataru Takeda
December 31, 2019	Complete and submit final report	Anne Ruckman

Budget Justification

Expense	Amount Requested	Justification
Lithium Carbonate	$400.00	1kg for sample preparations
Boric Acid	$100.00	1kg for sample preparations
Silica Powder	$200.00	1kg for sample preparations
Poster Materials	$150.00	SPS member poster presentations
Mentor/Mentee Introduction: SPS member pairing, research safety training, Dr. Bragatto's talk at Coe	$150.00	SPS mentors/mentees will discuss project goals, receive safety training, and Dr. Bragatto will talk about ionic conductivity testing
Iowa State University Trip	$600.00	10-15 SPS members will tour the Department of Materials Science and Engineering at Iowa State University and several will participate in analyzing lithium borate glass properties.
Dr. Martin's talk at Coe College	$300.00	Cost for transportation, lunch and light refreshments for Dr. Martin's trip to and lecture at Coe College.
Dr. Bragatto's talk at ISU	$100.00	Transportation costs

Besides the SPS funding, we are also pursuing financial assitance from:

- Coe College Student Senate with Society of Physics Students $400
- Coe College Physics Department-Lab space, mixing materials and furnaces $300
- Coe College Learning Commons Micro-Grant $200

Bibliography

[1] Varshneya, A. K. (1994). *Fundamentals of Inorganic Glasses*. Academic Press.

[2] Martin, S. W. (1991). Ionic Conduction in Phosphate Glasses. Journal of the American Ceramic Society, 74(8), 1767–1783.

[3] Montouillout, V., Fan, H., del Campo, L., Ory, S., Rakhmatullin, A., Fayon, F., & Malki, M. (2018). Ionic conductivity of lithium borate glasses and local structure probed by high resolution solid-sate NMR. Journal of Non-Crystalline Solids, 484(November 2017), 57–64.

[4] Charles, R. J. (1963). Some Structural and Electrical Properties of Lithium Silicate Glasses. *Journal of the American Ceramic Society*, *46*(5), 235–238.

[5] Voigt, U., Lammert, H., Eckert, H., & Heuer, A. (2005). Cation clustering in lithium silicate glasses: Quantitative description by solid-state NMR and molecular dynamics simulations. *Physical Review B - Condensed Matter and Materials Physics*, *72*(6), 1–11.