

# Proposed Summer 2021 Internship Position | Machine Learning and Molecular Simulations

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Desired Level: PhD student in Chemical Engineering, Materials Science or related field.

## Position Overview

The intern will join the modeling and scientific computing group within the Science and Technology (S&T) division and will support the development and application of new computational methods to study diffusion and electric-field induced ionic transport in oxide glasses. They will join the thermal poling project and will have the opportunity to collaborate closely with a multidisciplinary team of scientists in the modeling group, the process research group and the surface science and characterization group. They will be introduced to the fundamentals of glass science and engineering through mentorship and contributions to the Thermal Poling of Glass (TPG) project, a current project in the fundamental research portfolio at Corning.

## About the Project

Thermal poling is a process by which spatial rearrangement of ionic species is achieved within a multicomponent oxide glass at moderate temperatures through the application of an external electric field. This leads to the creation of a depletion layer near the anodic surface of the glass which exhibits different structure and properties compared to the parent glass. These changes can, in turn, be used to increase the value of various commercial Corning glasses through targeted surface engineering as well as the development of new processes to achieve them.

## Internship Goals

In this project, the intern will use various modeling techniques to develop fundamental understanding of the mode of ionic transport that take place in oxide glasses submitted to an external electric field. More specifically, the intern will work towards the followings:

- Explore the use of transition state theory to study the kinetics of ionic migration in oxide glasses
- Explore the use of machine learning coupled with molecular simulations in diffusion studies
- Analyze results to gather new insights into preferred electric-field induced migration pathways in oxide glasses
- Compare modeling findings with experimental results

## Internship Outcomes

The diffusion of network modifiers (charged ionic species) in oxide glasses is technologically relevant to numerous applications at Corning but the work that the intern will do will be fundamental enough to allow for an external publication at the end of the internship.