# Research Proposal

## Materials Modeling of Future Optical Devices: Gallium Nitride Nanoclusters Embedded in Silica Glass

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# Research Objective

Gallium nitride (GaN) is a semiconductor widely used in optoelectronic devices, such as blue lasers and light-emitting diodes (LEDs). [1] However, like many other substances, GaN is known to exhibit interesting optical and electronic properties when present in the nanoscale. [2] A strong theoretical understanding of the reasons for these properties will allow a great degree of control over the behavior of the new materials, as well as over possible side effects. Thus the goal of this project is a theoretical characterization of gallium nitride nanoclusters embedded in silica glass using computer modeling.

# Introduction

Many chemical compounds are known to exhibit unusual properties when present as very small entities. These unusual properties are often due to quantum effects, such as electron confinement, which are not apparent on a macroscopic scale. [2] A prime example of these effects at play is the unusual behavior of silicon, the primary substance in semiconductors. Solid blocks of silicon have no observed optical activity in the visible range. However a very different set of properties emerge when silicon is present as small, nanosize particles. These "nanoclusters" of silicon, having a diameter of less than $5\,\mathrm{nm}$, are known to be photoluminescent and are known to emit visible light if properly excited. [3] The wavelength, and consequently the color, of light emitted was theoretically shown to depend not only on the size of the cluster, but also on the interface between the cluster and the surrounding silica. [4] To further understand the quantum behaviour of nanocrystalline silicon in silica, the orbital structure of several clusters were elucidated on the basis of Density-Functional Theory (DFT) calculations. [5] In the study, a quantum confinement effect was observed in the nanocluster, as well as an interesting orbital structure on the interface betweeen the cluster and the surrounding silica.

Gallium nitride (GaN) is a semiconductor similar to silicon currently in wide use for various optoelectronic devices such as blue lasers and light-emitting diodes (LEDs). [1] Furthermore, the nanoclusters are known to be quite heat-resistant, making them ideal for high-temperature electronics [6]. While free nanoclusters of GaN are known to exhibit photoluminescent properties [7], little is known about the optical and electronic properties of gallium nitride nanoclusters embedded in silica. Thus, the thrust of this research is to explore, using theoretical computational tools, the optical and electronic properties of gallium nitride nanoclusters embedded in amorphous silica, as well as to understand on a fundamental level the electronic structures which give rise to those properties.

# Significance

A key factor in determining the application of new materials is a thorough understanding of its properties. If powerful theoretical tools for modeling and simulation are not fully exploited, many opportunities for discovery may be missed. Since free nanoclusters of gallium nitride demonstrate interesting optical properties, it is reasonable to expect GaN nanoclusters embedded in silica to do the same. Given a set of other superior properties, nanocrystalline GaN may be the future candidate for use in many electronic and optoelectronic devices.

Understanding the theoretical reasons for the properties will also allow a great degree of control over the behavior of the new materials (e.g. through metal doping), as well as over possible side effects. Thus the goal of this project is a theoretical characterization of gallium nitride nanoclusters using computational modeling.

## Methodology

In this study, the interface between amorphous silica and GaN nanoclusters will be investigated, with a particular emphasis on optical and electronic properties. The first step involves creation of the models using custom scripts and CrystalMaker. These structures will then be optimized using the Vienna *Ab-Initio* Simulation Package (VASP), a program designed for efficiently handling molecules and crystals at a quantum level.

Following optimization of the clusters, VASP will again be used to calculate the optical and electronic properties of the embedded nanoclusters. A map of several significant molecular orbitals such as the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) will also be calculated, as well as the band gap energy, a quantity of interest in solid-state physics and chemistry. We aim to establish relationships between the electronic structure of the nanoclusters and the properties they are expected to exhibit.

The creation of the clusters will be done locally using local computers. However, majority of the optimizations and property calculations will be executed on national supercomputers such as the Texas Advanced Computing Center (TACC) in Austin, Texas, or NASA supercomputing clusters.

## References


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