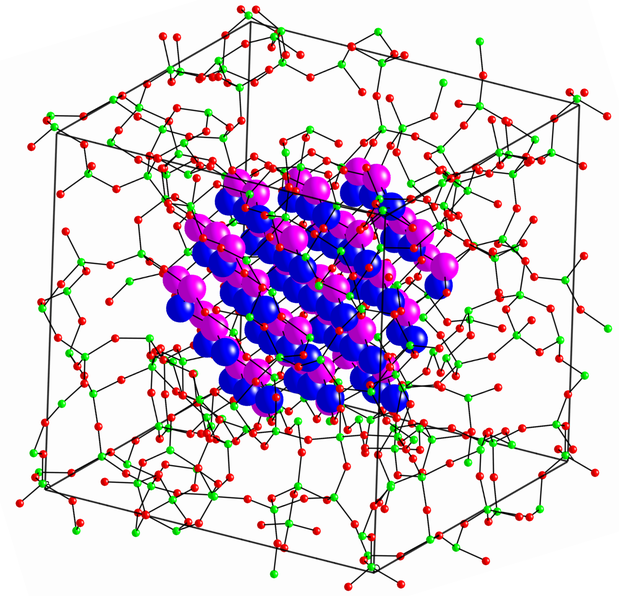
Materials Modeling of Future Optical Devices:
Gallium Nitride Nanoclusters Embedded in Silica Glass

Pinaki Bose and Peter Kroll

Department of Chemistry and Biochemistry
The University of Texas at Arlington

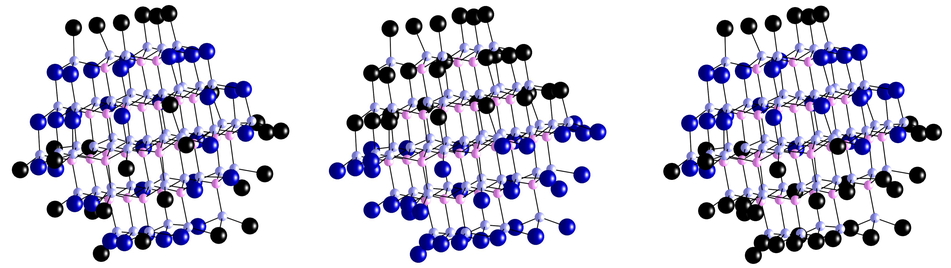
Motivation

- Gallium nitride (GaN) is a wide band-gap semiconductor which emits blue light
- Nanoclusters of GaN in silica (GaN@SiO2) are candidates for blue light emitting devices
- Computational studies for screening of properties and interface chemistry to support efficient synthesis



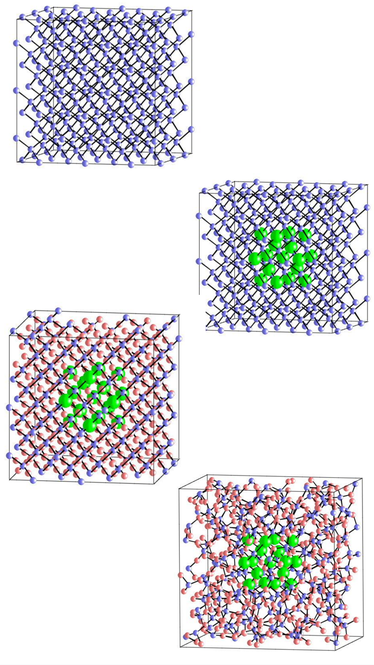
Interface Chemistry

Growth of nc-GaN can be homogeneous or along preferred facets. Charge balance requires the nanocluster-silica interface to have a mixture of N-Ga-O and N-Si-O bonds. Various patterns may occur.

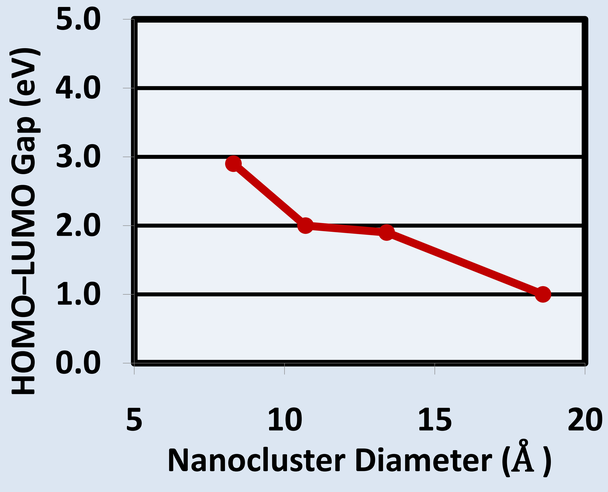


Nanocluster Construction

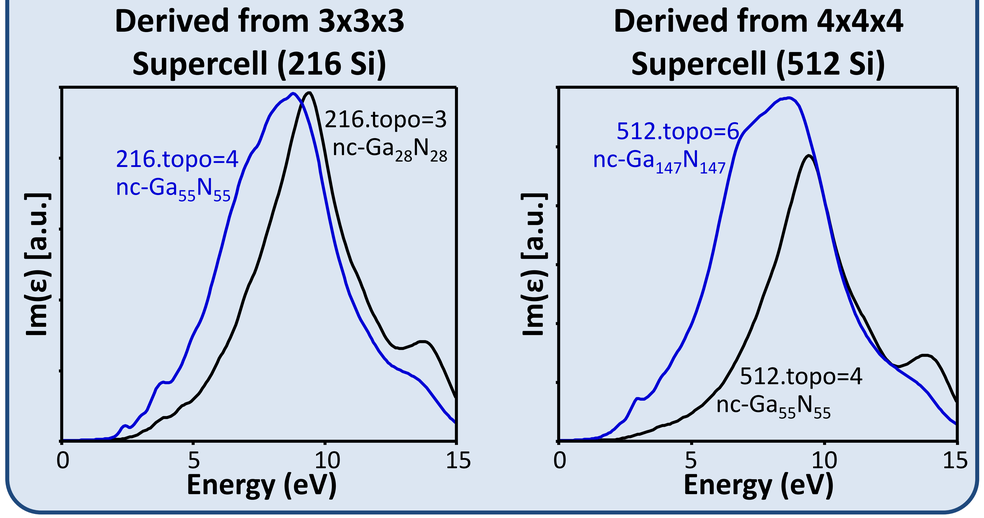
- Generate 3x3x3 supercell of sphalerite (216 atoms)
- Define core/nanocluster with fixed topological size
- Insert oxygens between non-core atoms → formation of oxide matrix
- Convert core cluster to GaN → GaN@SiO_2 (interface !)
- Randomize SiO_2 structure with Bond Switch algorithm
- Structure optimization using DFT (VASP)
- Calculate electronic and optical properties
- Repeat with a 4x4x4 supercell (512 atoms)



Band Gap Calculation



Dielectric Function



We thank the NSF for financial support (DMR-0907117) and the TACC for computational facilities (Lonestar and Ranger)