ZnO has numerous uses in electronics. For example, ZnO has been studied as a candidate material for use in LEDs, n-p junctions, and Al/Au ohmic contacts. There has been recent interest in Al-doped ZnO for its thermoelectric properties. This is because this material possesses a high Seebeck coefficient, which measures the electrical potential generated by applying a thermal (temperature) gradient. The structural stability at temperatures above 1300 °C allows ZnO to be used as a high-temperature thermoelectric generator.

ZnO nano-particles have been studied for photocatalytic applications. A photo-catalyst is used as a catalyst for a chemical reaction under certain lighting conditions. ZnO thin films can be used to degrade chemicals such as methyl blue into less toxic chemicals.

ZnO thin films have been studied for use as a fiber-optic temperature sensor, and it can also be used as a NH3 gas sensor. Au-ZnO thick films have been studied for use as an ethanol sensor. Various forms of ZnO with dopants or composites have been studied for use as a variety of bio-sensors. ZnO inverse opal electrodes have been studied for use as a glucose sensor. A ZnO based paste has been studied for use as a BPA sensor. A flower shaped ZnO nanostructure has been studied for detection of meningitis. ZnO has even been added to cellulose to study for increasing immune response.

More details of these works can be found in the project report.

**Method**

The primary tool used in this paper is the Vienna Ab Initio Simulation Package (VASP), which is based on the density functional theory (DFT) to calculate the ground-state property of a substance. There are three known phases of ZnO, namely wurtzite (W), rock salt (RS), and zinc blende (ZB). The initial step is to determine the transition pressure for the structural transformation between the ZnO phases. This helps set a clear distinction between the high-pressure and ambient-pressure calculations.

The second step is to obtain the bulk modulus. To calculate the bulk modulus, each structure is placed under a series of uniform pressure distortions applied to the lattice. By using the difference in energy between the distorted and undistorted structure, the elasticity of the structure can be calculated.

**Elastic Constants**

The ambient-pressure elastic constants for the W ZnO phase. Top Right: The high-pressure elastic constants for the W ZnO phase. Bottom Left: The ambient-pressure elastic constants for the RS & ZB phases. Bottom Right: The high-pressure elastic constants for the RS & ZB phases. The distortions used were kept small to keep the change in volume small. The dashed lines are the results of linear fits. These linear fits are used to extrapolate the elastic constants for 0% distortion.

**Results & Discussion**

**Transition Pressure & Bulk Modulus**

The transition pressure from Figure 1 gives a clear distinction between high and low pressure calculations. The high pressure calculations were done at 15 GPa. By using a direct derivative method, we calculated the bulk modulus for the high pressure ZnO structures. The resulting bulk moduli are 193, 229, and 192 GPa for the W, RS, and ZB phases, respectively.

**Conclusions & Further Study**

The present work predicts a structural transition from the wurtzite to RS phase of ZnO at 11 GPa. We therefore performed high-pressure calculations at 15 GPa. The bulk moduli for the ambient-pressure structures are within 5% of previously reported results. Our calculations indicate that the high-pressure bulk moduli of ZnO phases increase between 38% and 50%. The RS and ZB phases of ZnO show increasing values of elastic constants C11 and C12 at higher pressure, while the value of C13 decreases at higher pressure. On the other hand, the wurtzite phase shows all increased elastic constants with increasing pressure. A comparison was made between the elastic constants of the ZnO phases and those of silicon. With the exception of C13 and C12 in the wurtzite phase, the three phases of ZnO exhibit higher values of elastic constants, indicating their higher strength under structural deformation. An important topic for future study of ZnO is to explore the electronic band structure and phonon dispersion, which will determine the properties crucial in many device applications. The structural results obtained in this work have laid a key foundation for continued research.