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 photocatalyst 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.

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 C66 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 C55 and C66 in the wurtzite phase, the other constants of ZnO are higher than those of silicon. The high-pressure elastic constants for the W ZnO phase. The ambient-pressure elastic constants for the W ZnO phase. The high-pressure elastic constants for the RS & ZB phases. The ambient-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.

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 values. The resulting energy data are then fitted against the Birch-Murnaghan Equation of States (EOS). The third step is to calculate the elastic constants. The W structure is a hexagonal closely packed lattice. The RS and ZB phases have cubic lattices. To calculate the elastic constants, distortions are applied to the lattice. By using the difference in energy between the distorted and undistorted structure, the elasticity of the structure can be calculated.

The purpose of this study is to determine structural and mechanical properties of zinc oxide (ZnO) using first-principles computational methods. ZnO is a semiconductor widely used in many electronic and optical applications. ZnO is also economically and environmentally desirable – first, both the constituent elements are abundant on Earth and therefore inexpensive for large-scale applications; second, it is non-toxic. The most significant contribution of this study is the simulations of the high-pressure phases. These high-pressure simulations are important because the rock salt phase of ZnO obtained at high pressure can be recovered at ambient pressure, and this new structural phase possesses different properties that may be more useful for certain applications.

Several past studies have been referenced for the present work. The first such study calculated the elastic constants using the computer code CRYSTAL98 [Orlando R, Dovesi R, Uguleno P, Roettig C, and Saunders VR, International Journal of Inorganic Materials, Vol. 1, 147-155 (1999)]. The second study for comparison obtained the elastic constants using the DFT package ABINIT [Duan Y, Qin L, Tang G, and Shi L, The European Physical Journal B, Vol. 66, 201-209 (2008)]. The third study for comparison obtained the elastic constants using the DFT package WIEN2k [Mohammadi AS, Biazeck SM, and Salehi H, World Applied Sciences Journal, Vol. 14, 1530-1536 (2011)]. While the elastic constants are the main focus of this study, there is a multitude of publications on ZnO that address its potential uses in many other areas of science and technology. In the next box on the right, we list several other applications of ZnO.

### Literature Review

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 values. The resulting energy data are then fitted against the Birch-Murnaghan Equation of States (EOS). The third step is to calculate the elastic constants. The W structure is a hexagonal closely packed lattice. The RS and ZB phases have cubic lattices. To calculate the elastic constants, distortions are applied to the lattice. By using the difference in energy between the distorted and undistorted structure, the elasticity of the structure can be calculated.

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