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.

The high-pressure elastic constants for the W ZnO phase. 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.

Figure 2. Top Left: 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 elastic constants of ZnO show increasing values of elastic constants C₁₁ and C₁₂ at higher pressure, while the value of C₃₃ 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 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 by 25% and 50% for the RS and ZB phases, respectively. The high-pressure geometry of ZnO structure is more compact compared to the ambient-pressure structure. The high-pressure RS ZnO structure can be recovered at ambient pressure. Right: The energies for the RS & ZB phases are plotted relative to the W phase energy. The crossover indicates a transition pressure of 11 GPa. At low pressures the W phase is more stable. At high pressure the RS phase is more stable. The high-pressure RS ZnO structure can be recovered at ambient pressure. Right: The energies for the RS & ZB phases are plotted relative to the W phase energy. The crossover indicates a transition pressure of 11 GPa. At low pressures the W phase is more stable. At high pressure the RS phase is more stable.

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 moduli 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 by 25% and 50% for the RS and ZB phases, respectively. The high-pressure geometry of ZnO structure is more compact compared to the ambient-pressure structure. The high-pressure RS ZnO structure can be recovered at ambient pressure. Right: The energies for the RS & ZB phases are plotted relative to the W phase energy. The crossover indicates a transition pressure of 11 GPa. At low pressures the W phase is more stable. At high pressure the RS phase is more stable. The high-pressure RS ZnO structure can be recovered at ambient pressure. Right: The energies for the RS & ZB phases are plotted relative to the W phase energy. The crossover indicates a transition pressure of 11 GPa. At low pressures the W phase is more stable. At high pressure the RS phase is more stable.

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