ABSTRACT

Beryllium chalcogenides semiconductors are technologically significant because of their wide applications in light-emitting devices, detection systems for environmental pollution and color-displaying modules. There has been an increasing interest in the study of Beryllium chalcogenides under high-pressure conditions, driven by the need of synthesizing new solids with targeted physical properties such as elastic constants electrical and electronic properties. Previous studies indicate that there are discrepancies in the calculated values of phase transition pressures lattice parameters and elastic constants. An *ab initio* study was undertaken to determine the phase transition pressures, lattice parameters, and elastic properties of beryllium chalcogenides. All calculations were done using an open source quantum ESPRESSO code. The results from the phase transition study indicate that; $B3 \rightarrow B8$ was at 56.5GPa, 51.5GPa and 38.5GPa for $B1 \rightarrow B8$ the transition took place at 54.5GPa, 44.5GPa, and 34 GPa for BeS, BeSe and BeTe respectively. The calculated values of the lattice parameters and other mechanical properties agreed within the 10% accuracy with respect to experimental values. The results therefore points out the fact that the B3 crystal structure is the most stable phase in the three compounds at 0GPa.