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Structural and Elastic Properties of MgX (X=Se, Te) Semi Conducting Compounds under High Pressure

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Abstract: In the present paper, we have investigated the high-pressure structural phase transition of magnesium chalcogenides using the three-body potential (TBP) model. Phase transition pressures are associated with a sudden collapse in volume. The phase transition pressures and associated volume collapses obtained from TBP are in reasonably good agreement with experimental data. In addition, the elastic constants and their combinations with pressure are also reported. It is found that TBP has promise to predict phase transition pressure, elastic constants, and their pressure derivatives for other chalcogenides as well.

Key Words: Alkaline earth chalcogenides, phase transitions, high-pressure

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