

Analysis of Structural Phase Stability of Strontium Sulphide under High Pressure

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Abstract : A Three Body Interaction Potential (TBIP) model is developed to study the high pressure phase transition of SrS having NaCl (B1) structure at room temperature. This model includes the long range Columbic, three body interaction forces, short range overlap forces operative up to next nearest neighbors and zero point energy effects. We have investigated the phase transition with pressure, volume collapse and second order elastic constants and found results well suited with available experimental data.

Keywords : phase transition, second order elastic constants, three body interaction forces, volume collapses

Conference Title : ICPE 2015 : International Conference on Physics Education

Conference Location : Singapore, Singapore

Conference Dates : September 10-11, 2015