

Abstract Submitted
for the TSF05 Meeting of
The American Physical Society

Pressure-Induce phase transition of ZnS ISRAEL MARTINEZ, MURAT DURANDURDU, Department of Physics, University of Texas at El Paso — We study the pressure-induced phase transition of ZnS using an ab initio constant pressure technique. The transition from the zinc-blende structure to a rocksalt structure is successfully reproduced through the simulation. The transformation mechanism is characterized and found that the transformation is due to the monoclinic modification of the simulation cell, similar to that found in SiC. [1, 2]. Furthermore, our finding supports the universal transition state of high-pressure zinc-blende to rocksalt transitions [3].

References:

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Date submitted: 15 Sep 2005

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