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Structural phase transition of GeTe under pressure GAP-SOK DO, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology, Pohang 790-784 — Structural phase transition of a representative chalcogenide semiconductor, GeTe, is studied with the use of ab initio pseudopotential density functional method. The transition pressure and atomic structures are particularly investigated. By fitting calculated energy-volume data with Birch-Murnaghan equation, we obtained a transition pressure of 3.7 GPa for rhombohedral to NaCl structural transition and 42 GPa for NaCl to CsCl transition, which is in an excellent agreement with experiment [1, 2]. Other structures are also studied for possible transitions at intermediate pressures. The role of Te d orbitals is discussed in regard to the transition pressure and cohesive energy.

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[2] N. R. Serebryanaya, V. D. Blank, V. A. Ivdenko, Phys. Lett. A 197, 63 (1995)

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