

Abstract Submitted
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Quasi-particle spectra of various forms of crystalline Germanium Telluride JINWOONG KIM, Department of Physics, Pohang University of Science and Technology, GEUNSIK LEE, Department of Physics, University of Texas at Dallas, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology — GeTe is known to undergo a very complex structural phase transition under pressure. Also it changes the phase upon heating from crystalline NaCl structure to amorphous phase. Several models were suggested for possible structural transition pathways such as Toledano, Modified Buerger and Watanabe model. We have investigated the dielectric function of GeTe at representative structural phases using the pseudopotential density functional method within the generalized gradient approximation. To calculate the quasiparticle spectra, we carried out the GW calculations. Semicore d-electrons of Te are found to be very critical for calculating correct transition pressures, and they are included explicitly as valence. These electrons affect the electronic structures through the p-d coupling, which is found non-negligible. Our results can help analyze experimental data and investigate the transition pathway of GeTe.

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