

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Consequences of ionic and covalent bonding in Ge-Sb-Te phase change materials** SAIKAT MUKHOPADHYAY, Materials Science and Technology Division, Oak Ridge National Laboratory, JIFENG SUN, Department of Physics and Astronomy, University of Missouri, ALASKA SUBEDI, Max Planck Institute for the Structure and Dynamics of Matter, THEO SIEGRIST, Department of Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, Tallahassee, DAVID SINGH, Department of Physics and Astronomy, University of Missouri — Structural transformation of  $\text{Ge}_2\text{Sb}_2\text{Te}_5$  has attracted a great deal of research as it involves two states (crystalline and amorphous) that are stable at ambient temperature but with remarkably different physical properties, in particular, very different optical constants. The differences in physical properties in these states have been explained in terms of resonant bonding that has been generalized to the description of covalent systems with high symmetry structures such as benzene and graphite. However, given the local lattice distortions noted from both experimental and theoretical investigations, it is clear that the meaning of “resonant bonding” in GST is very different from that in graphite or benzene and the precise nature of bonding in this phase has not been fully established. In this talk, based on our first-principles calculations, we show that there is a strong competition between ionic and covalent bonding in the cubic phase, and establish a link between the origins of phase change memory properties and giant responses of piezoelectric materials.

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Date submitted: 05 Nov 2015

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