**Case Study Summary-Jason Larkin: Molecular Modeling of Phase Change Alloy GeTe**

This case study will review the current state of research concerning the molecular modeling of a class of semiconductor alloys called phase change materials. In particular, the alloy GeTe will be the focus [3]. Quantum mechanical methods have been the primary modeling tool for GeTe. Studies using these methods will be discussed and reviewed [1,2,4,5]. The potential for classical Molecular Dynamics modeling of GeTe will also be discussed.

**References**

## [1] J. Akola, R.O. Jones Phys. Rev. Lett. 100, 205502 (2008).

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[3] A V Kolobov et al.,2004J. Phys.: Condens. Matter16 S5103.

## [4] K. M. Rabe, J. D. Joannopoulos Phys. Rev. B 36, 3319–3324.

## [5] J. Y. Raty et al., Phys. Rev. B 65, 115205 (2002).