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

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