Phase Change Materials for Non-Volatile Memories : Properties and Optimization through Ab Initio Simulation

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Phase Change Materials are emerging as active components of non-volatile memories thanks to their ability to switch extremely rapidly from a conducting crystal to a more semiconducting glassy. Using Ab Initio simulations, we address the structure and some properties of the glassy phase, like aging, but also go back to the description of bonding in the crystalline phase.

We develop a two-dimensional map based on a quantum-topological description of electron sharing and electron transfer in binary solids. This map intuitively identifies the fundamental nature of ionic, metallic, and covalent bonding in a range of elements and binary materials. Furthermore, it highlights a distinct region where phase change materials are found and for which bonding has been qualified as 'metavalent' [1,2]. Extending this map into the third dimension by including physical properties of application interest, we show that bonding in metavalent compounds differs from the our usual views of bonding. This map could be used to help designing new materials: by searching for desired properties in a 3D space and then mapping this back onto the 2D plane of bonding.

[1] J.Y. Raty, M. Schumacher, P. Golub, V. Deringer, C. Gatti and M. Wuttig Advanced Materials, (2018) 1806280
[2] M. Wuttig, V. Deringer, X. Gonze, C. Bichara and J.Y. Raty, Advanced Mater. (2018) 1803777
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