

Allgemeines Physikalisches Kolloquium

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Phase change materials for data storage: insights from atomistic simulations

Telluride materials such as the GeSbTe ternary alloys or the GeTe compound have been deeply investigated over the last two decades for a wide range of applications ranging from optical disc (DVDs and Blu-ray disc) to non-volatile electronic memories (phase change memories, PCM) and neuromorphic computing.

These applications rest on a reversible and very rapid (50 ns) transformation between the amorphous and crystalline phases upon heating due to laser irradiation in the optical disc or to Joule effect in the electronic memories. The encoding of the digital information exploits a large difference in the optical reflectivity or in electronic conductivity between the two phases. Materials in this class, named phase change materials, feature a very rich portfolio of intriguing properties that make them suitable for application in the different data storage devices.

In the Colloquium I will review our contribution to the microscopic understanding of the functional properties of phase change materials that we gained from atomistic simulations either based on electronic structure calculations within Density Functional Theory or from large scale molecular dynamics simulations based on machine learning techniques.