GOING DEEPER ON THE STRUCTURAL AND ELECTRONICAL PROPERTIES OF AMORPHOUS GE_XSE_{1-X}: A MICROSCOPIC INVESTIGATION

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Amorphous chalcogenides, such as Ge_xSe_{1-x}, have been proposed as good ovonic switch material candidates for nonvolatile memory and selector devices due to their fast switching, endurance and higher crystallization temperature with respect to standard GST compounds. The structural and electrical properties of Ge_xSe_{1-x}, as for other chalcogenides, are strongly related to the presence of short- and medium-range structures in the amorphous phase that are responsible for the internal structural orders at different length-scales.[1][2]. In order to deeply understand the local geometry-dependent properties of these chalcogenides systems, we employed a combined approach based on both classical molecular dynamics (MD) simulations and density functional theory calculations.

To obtain a deep insight into the structural features of Ge_xSe_{1-x} systems at the atomistic scale, MD simulations have been employed to study Ge_xSe_{1-x} systems containing thousands of atoms and simulated for hundreds of nanoseconds. The obtained structures were accurately analyzed using cutting edge techniques and theories based on the chemical/physical and topological approaches shedding light on how the different percentages of Ge and Se affect the order at different lengths.

In order to compute the electronic properties of amorphous Ge_xSe_{1-x} systems, we developed a procedure to extract several configurations of few hundreds of atoms from the extended structures obtained from MD simulations. The results show that a small difference in the stoichiometry affects not only the mobility band-gap size, but also the number and the position of the trap states with respect of the mobility edges.

Using both approaches, MD and quantum simulations, we obtained different information about the nature of the order in these systems demonstrating that little changes in the stoichiometry greatly affect the Ge_xSe_{1-x} structural and electrical properties.

References

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