Device to materials pathway for electron traps detection in amorphous GeSe-based selector

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Choosing the ideal material employed in selector devices is a challenging task from the theoretical and experimental side [1], mainly due to the need for a synergistic approach between techniques. We propose a material-to-device multiscale technique [2] (including experiments, device modelling, and atomistic simulations) that extracts traps/defects characteristics from the experimental device electrical data and connect them to the microscopic properties of the materials (atomic defect), in a learning that correlates the electrical properties of the specific device to the electronic properties. We use this material-to-device multiscale technique for the efficient characterization of active traps of amorphous GeSe chalcogenides, being able to trace back the specific features of materials responsible for the measured findings and to connect them with an atomistic description of the sample. We will describe the overall approach, focusing on the Density Functional Theory calculations that are part of this workflow. We find that hole and electron trap states have different characteristics: the former do not exhibit the presence of homopolar Ge-Ge bonds that are, instead, a common feature of the latter. Our combined approach can be applied to other materials and devices, which is very beneficial for the efficient development and optimization of existing and novel technologies.

References

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