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Conductivity in amorphous chalcogenides. KIRAN PRASAI, Ohio University, PARTHAPRATIM BISWAS, The University of Southern Mississippi, DAVID DRABOLD, Ohio University — Metal doped glassy chalcogenides show swift change in conductivity in response to a small external voltage and are being used to make memory elements. We study here the microscopic origin of such conductivity in a canonical material of this category: (GeSe3)xAg100-x. We have used a novel method to electronically design the conducting phase of this material via a biased ab initio MD simulation. We briefly discuss the modeling technique here. We study the models and point out the structural and electronic features of the conducting phase and draw the contrast with their insulating counterparts. We also point out the role of silver clusters/wires in the conductivity by an explicit simulation of such structures with the glassy matrix.

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