

Abstract Submitted
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**Atomistic Picture of the Intermediate Phase in GexSe_{1-x} Glasses:
A Joint Theoretical and Experimental Study¹** FAKHAR UL INAM, GANG
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DRABOLD, Ohio University — Raman and calorimetric studies on GexSe_{1-x}
glasses have provided evidence for the existence of the intermediate phase (IP) in
chalcogenide and other glasses. Here, Ab-initio molecular dynamics (MD) based
models of these glasses are discussed, and an atomistic picture of the IP, based
upon the models and available experiments, is presented. A thorough analysis of
our models reveals that the IP in GexSe_{1-x} glasses appears due to the competition
between the percolating GeSe_2 phase and the a-Se phase, which gives rise to the
“flattening” of the observables in the IP window. We present X-Ray Absorption
Near Edge Structure (XANES) measurements on germanium selenide glasses in the
IP composition range, and detect an electronic signature of the IP in terms of the
shift of the XANES white line (WL) and non-linear behavior of their intensities in the
IP window. We show that these models appear to properly represent the XANES
results.

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