

Simulation of liquid and amorphous Germanium diselenide surfaces

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The structure of the surfaces of liquids and glasses is an open frontier, especially for simulations. It is difficult to apply standard experimental techniques such as scanning tunneling microscopy to determine the atomistic structure at the surfaces. We study the binary chalcogenide GeSe_2 in the liquid and amorphous phase in a slab geometry. We study the structure and dynamics at the surfaces and we quench the liquid in the slab geometry to form surfaces of the amorphous phase. Detailed comparison with previous theory and experiment is provided.