Abstract Submitted
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Molecular-Dynamics (MD) Simulations of Copper Diffusion in Copper Chalcogenides JING WANG, None — It was recently discovered that copper chalcogenides Cu2S and Cu2Se are viable candidates for thermoelectric materials with high figure of merit (ZT) values at temperatures around 1,000 K [1,2]. And the possible reason for the high ZT is the low thermal conductivity arising from liquid-like Cu atoms in those phases. In this work, we perform first-principles molecular dynamics simulations to study the motion of Cu atoms in the high-temperature phases of Cu2S and Cu2Se and confirm the liquid nature of Cu atoms. To get a better understanding of the diffusion patterns of the systems, we have examined all the three phases of Cu2S (monoclinic, hexagonal and cubic phases with increasing temperature). Starting from the hexagonal phase the Cu atoms show a disordered/liquid-like feature with a jump diffusion pattern. We find that the diffusion is faster in x-y directions than in the z direction. A more isotropic diffusion pattern is found for high-temperature cubic phase with a much larger diffusion coefficient.1] Y. He et al. Adv. Mater. 26, 3974 (2014) 2] H. L. Liu et al. Nat. Mater. 11, 422 (2012)

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None

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