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Ab Initio Study of Phase-Change Materials Doped with magnetic Impurities RICCARDO MAZZARELLO, YAN LI, RWTH Aachen University — Chalcogenide Phase-change materials are of great technological importance due to their ability to undergo reversible and fast transitions between the amorphous and crystalline phases upon heating. Recently, it was shown experimentally that $Ge_2Sb_2Te_5$ doped with Fe atoms exhibits phase-change behavior for low concentrations of Fe and that both the amorphous and the crystalline phases are ferromagnetic at low enough temperatures. Moreover, the two phases were found to have different saturation magnetization. This finding opens up the possibility of exploiting the phase-change behavior for fast magnetic switching in e.g. spintronic devices. We have investigated the structural, electronic and magnetic properties of Fe-doped $Ge_2Sb_2Te_5$ by first-principles simulations based on Density Functional Theory. Both amorphous and crystalline (hexagonal and cubic rocksalt) phases of $Ge_2Sb_2Te_5$ were considered. Our results show that in the amorphous phase, the magnitude of the magnetic moments of the Fe impurities is reduced with respect to the crystalline phases, due to the different local geometries and chemical environments, which explains the experimentally observed magnetic contrast between the two phases.

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