Supplementary material for:
The role of vacancies and local distortions in the design of new phase change materials

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In the manuscript “The role of vacancies and local distortions in the design of new phase change materials” we discuss the removal of Ge and Sb atoms from “GeSbTe” alloys. Their removal significantly reduces the total energy and is thus favoured by the system. If Te vacancies are considered too, the situation changes qualitatively because removal of 2 Te atoms increases the energy by more than 3 eV (data not shown). Hence Te vacancies are unfavourable in the ideal rocksalt structure. A similar finding has been reported for GeTe where Te vacancies were also much less favourable than Ge vacancies¹. The situation changes, however, if local distortions of the Ge₂Sb₂Te₄ crystal are allowed. Then, the system reduces its energy drastically by moving an adjacent Ge atom into the Te vacancy. This produces an antisite defect, where the Ge atom forms a homopolar bond to a Ge neighbour. The formation energy of this defect is quite low. Thus homopolar bonds are very likely to occur in defect-rich structures such as the amorphous phase. Since these defects have formation energies that are nevertheless higher than the formation energies of Sb and Ge vacancies, we do not consider these Te antisites for the rocksalt-like crystalline phase.
in the manuscript.
