

Supporting Information

**First-principles thermal transport
in amorphous Ge₂Sb₂Te₅ at the nanoscale**

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1. Pseudopotentials

The pseudopotentials used for Ge (file Ge_MT_BLYP.psp), Sb (file Sb_MT_BLYP.psp) and Te (file Te_MT_BLYP.psp) can be downloaded at the url:

<https://www.cpmd.org/wordpress/index.php/documentation/pseudo-potentials/>

2. Atomic configurations

The atomic coordinates of models D, D2 and D4 are available in XYZ format in the files D.xyz, D2.xyz and D4.xyz.