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First principles study of crystalline and amorphous Ge2Sb2Te5 and the effects of stoichiometric defects

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Corrigendum

First principles study of crystalline and amorphous Ge₂**Sb**₂**Te**₅ **and the effects of stoichiometric defects** S Caravati, M Bernasconi, T D Kühne, M Krack and M Parrinello 2009 *J. Phys.: Condens. Matter* **21** 255501

Figure 11 reporting the projections of the electronic density of states on s, p and d pseudowavefunctions was actually obtained from an orthogonalized set of pseudowavefunctions and did not follow the definition given in section 2 of the paper. The correct projections are reported in the revised figure below. The contribution from d wavefunctions is negligible on the scale of the figure and has been omitted.

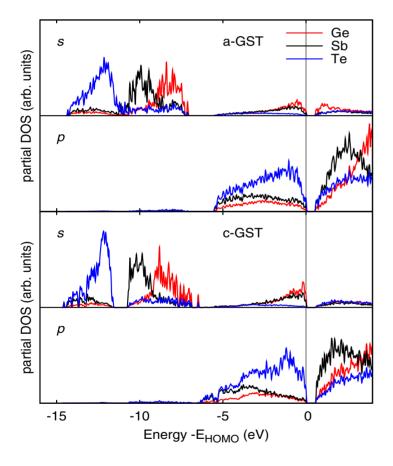


Figure 11. Electronic density of states of the stoichiometric a-GST and c-GST models projected on atomic s and p pseudowavefunctions.