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Supplementary material: Unraveling the role of chemical composition in the lattice thermal conductivity of oxychalcogenides as thermoelectric materials assisted by machine learning.[†]

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Oxychalcogenides represent a large chemical space with potential application as thermoelectric materials due to their low thermal conductivity. However, the nature of this behaviour is still under debate. Understanding the origin of the anharmonicity of these materials is key to developing models that improves the efficiency of thermoelectric materials. In this work, we combine machine learning with first principles calculations to explore oxychalcogenides materials. Machine learning not only accelerates the prediction of the lattice thermal conductivity for large chemical spaces with high accuracy, but also catalyzes the development of design principles to discover new thermoelectric materials. Using this approach, lattice thermal conductivity has been directly connected to the effect of each species in the material, using atomic projections of the scattering rates. The role of the the monovalent atom and the lone pair electron for the trivalent cation are discussed in detail. Based on this knowledge, it is possible to connect complex properties such as lattice thermal conductivity with a more manageable synthetic variable such as chemical composition. Using this strategy, we propose promising new oxychalcogenides such as BioAgSe, which subsequently has been confirmed as having ultra-low lattice thermal conductivity.

Author Contributions

The authors confirm contribution to the paper as follows: Conceptualization: J.J.P. and A.M.M.; Data curation: E.J.B and J.S.; Investigation: E.J.B, J.S. and F.L.P.; Visualisation: E.J.B.; Writing – original draft: J.J.P.R., A.M.M. and J.F.S. All authors reviewed the results and approved the final version of the manuscript.

Conflicts of interest

There are no conflicts to declare.

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Notes and references

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Fig. 1 (a) Convergence of κ_l and the root-mean-square error, RMSE, of the fitted forces with the number of distorted structures used to obtain force constants in comparison with the value reported using a full-DFT approach.¹ The shaded area represents deviations of ±5%. (b) Convergence of κ_l with the **q**-points grid size used in the BTE.



Fig. 2 (a) Phonon dispersion curves for BiOCuS. (b) Phonon group velocities for BiOCuSe and BiOCuS



Fig. 3 Phonon dispersion curves for $BiOAg_{0.5}Cu_{0.5}Se$ at 0, 100, 200, and 300 K.