Electronic Supplementary Information

Anharmonicity and ultralow thermal conductivity in layered Oxychalcogenides BiAgOCh (Ch=S, Se, and Te)

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Fig. S1. Calculated Hall coefficients of BiAgOCh (Ch=S, Se, and Te) as a function of temperature. They are initially extreme, lower with raising the temperature, and eventually approach to approximately zero.



FIG. S2. Calculated the three-acoustic phonon Grüneisen parameters and lifetime for (a,b) BiAgOS, (c,d) BiAgOSe, and (e,f) BiAgOTe.



FIG. S3. Calculated band structures for (a) BiAgOS, (c) BiAgOSe, and (e) BiAgOTe.



FIG. S4. Calculated density of states for BiAgOS, BiAgOSe, and BiAgOTe. Shadow region highlights the DOS peak of the delocalized p electrons from BiAgOSe.