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Phonon dispersion relations of Sb2S3 and Bi2S3 using the supercell force-constant method CHEE KWAN GAN, Institute of High Performance Computing, KUN TING EDDIE CHUA, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA, YUN LIU, Institute of High Performance Computing — We present a lattice dynamical study on the orthorhombic antimony sulphide (Sb_2S_3) [1] and bismuth sulphide (Bi_2S_3) [2] using the supercell force-constant method. We find that the slow decay of the interatomic force constants for these compounds in the Pnma setting critically demand the use of a large supercell of $2 \times 4 \times 2$ that consists of 320 atoms. To enable a practical calculation the space group information is fully utilized where only inequivalent atoms within the primitive cell are displaced for the force calculations. The effect of Born effective charges is incorporated into the method. We compare our results with that obtained from the density-functional perturbation theory. We found that smaller supercells could lead to unphysical acoustic phonon softening and lifting of the degeneracies along high symmetry directions. Our results provide a proper guideline for the use of the supercell force-constant method: the supercell size must be carefully be tested along with other parameters such as the kinetic energy cutoff, the Brillouin zone sampling or the self-consistent convergence criteria. [1] Y.Liu, K.T.E. Chua, T.C. Sum, and C.K. Gan, PCCP 16 (2014) 345. [2] Y. Zhao, K.T.E. Chua, C.K. Gan, J. Zhang, B. Peng, Z. Peng, and Q. Xiong, Phys. Rev

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