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Vibrational dynamics of filled skutterudites $M_{1-x}\mathbf{Fe_4Sb_{12}}$ (M = Ca, Sr, Ba, and Yb) ANDREAS LEITHE-JASPER, MPI for Chemical Physics of Solids, Dresden, MICHAEL MAREK KOZA, HANNU MUTKA, Institut Laue Langevin, Grenoble, France, WALTER SCHNELLE, HELGE ROSNER, YURI GRIN, MPI for Chemical Physics of Solids, Dresden — First-principles density-functional theory and lattice-dynamics calculations were performed to study the vibrational dynamics and related observables of the ternary compounds $M_{1-x}Fe_4Sb_{12}$ (A = Ca, Sr, Ba, Yb). The calculation results are supported by experimental data, which were obtained from neutron inelastic scattering, neutron-diffraction, and heat-capacity measurements. Within the calculation approach based on the theory of harmonic solids all observables are linked to the phonon density of states $Z(\omega)$. The good agreement with experimental data shows that the vibrational dynamics of the ternary skutterudite structures can be described by a set of normal modes. Features in the experimentally obtained density of states $G(\omega)$ reflecting the variation in properties (mass, ionic radius) of the cations Ca, Sr, Ba, and Yb are reproduced by the calculations.

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