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Lattice Dynamics of $FeMnP_{0.5}Si_{0.5}$ Compound from First Principles Calculation

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Understanding the role of lattice vibrations on first-order magnetic transitions is essential for their fundamental description, as well as for the optimization of the related functional properties. Here, we present a first principles study on the lattice dynamics of the $MnFeP_{0.5}Si_{0.5}$ compound. The phonon spectra are obtained by Density Functional Theory (DFT) calculations in combination with frozen phonon method. DFT calculations reproduce most of the features observed in experiments including the lattice softening across the magnetic phase transition and the pronounced shift of phonon peak. The site projected phonon density of states (pDOS) shows that the local vibrations of Mn atoms have an essential contribution to the overall lattice softening. Moreover, the local lattice vibrations of Mn atoms are rather featureless in the paramagnetic state (PM) and thus the total pDOS evolution across the transition appears to be dominated by Fe. The lattice vibrations of both Fe and Mn in the PM state are very sensitive to the local environment, which shows that the magnetic order and the local chemical environment are strongly coupled in this compound.

Key words: Lattice dynamics; Magnetic phase transition; Phonon softening; First principles calculation;