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Spin-phonon coupling effect in AMnO$_3$ (A=Ca, Sr, Ba) and LaMO$_3$ (M=Cr, Fe, Cr/Fe) from DFT+U and hybrid functional methods JIAWANG HONG, Rutgers University, ALESSANDRO STROPPA, CNR-SPIN, Italy, JORGE INIGUEZ, ICMAB-CSIC, Spain, SILVIA PICOZZI, CNR-SPIN, Italy, DAVID VANDERBILT, Rutgers University — Spin-phonon coupling effects, as reflected in phonon frequency shifts between ferromagnetic (FM) and G-type antiferromagnetic (AFM) configurations in cubic $CaMnO_3$, $SrMnO_3$, $BaMnO_3$, $LaCrO_3$, $LaFeO_3$ and $La_2(CrFe)O_6$, are investigated using density-functional methods. The calculations are carried out using the DFT+U method with a U that has been extracted by comparing with hybrid-functional (HSE) calculations. The phonon frequency shifts $\Delta\omega = \omega_{\rm AFM} - \omega_{\rm FM}$ obtained in this way agree well with those computed directly from the more accurate HSE approach, but are obtained with much less computational effort. We find that in the AMnO$_3$ materials class with (A=Ca,Sr,Ba), the Γ (R) phonon frequency shift $\Delta\omega$ decreases (increases) as the A^{2+} size increases. In LaMO$_3$ (M=Cr, Fe, Cr/Fe), the phonon frequencies at Γ decrease as spin order changes from AFM to FM for $LaCrO_3$ and $LaFeO_3$, but they increase for double perovskite $La_2(CrFe)O_6$. We discuss the prospects for bulk and superlattice forms of these materials to be useful as multiferroics.

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