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Phononic Structure Relationships in the Subgroup Phases of Ferroelectric $Ca_3Mn_2O_7$ ELVIS SHOKO, EMAN AL DAWOOD, UDO SCHWINGENSCHLOGL, PSE Division, KAUST, Saudi Arabia — The Ruddlesden-Popper (RP) compound, $Ca_3Mn_2O_7$, exhibits hybrid improper ferroelectric (FE) behavior in its $A2_1am$ phase. However, a new phase (space group $Acaa$), co-existing with the FE phase (200-320 K) and exhibiting negative thermal expansion (NTE) was recently discovered. This discovery highlighted the complexity of the phase relationships in the subgroup structure of $Ca_3Mn_2O_7$. Successful exploitation of RP compounds for FE applications depends on a clear understanding of the phononic relationships among the different relevant subgroup phases. Accordingly, we have used density functional theory (DFT) to map out the total energy landscape for the principal subgroup phases relative to the tetragonal phase. In order to elucidate the interrelationships of the soft phonon modes among the different subgroup phases, we performed lattice dynamics and quasi-harmonic approximation calculations. In addition, the latter calculations enabled us to extract mode Gruneisen parameters leading to new insights into the NTE behavior of $Ca_3Mn_2O_7$. The implications of our findings are discussed in the context of the potential of RP compounds as FE materials.

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