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Tuning ferroelectric polarization in $AA'\mathbf{MnWO_6}$ double perovskites through A cation substitution JOSHUA YOUNG, Drexel University, JAMES RONDINELLI, Northwestern University — Magnetic ferroelectric materials, which exhibit simultaneous magnetic and electric polarizations, have generated significant interest for application in novel electronic devices. Recent experimental work has shown that the double perovskite $NaLaMnWO_6$ exhibits anti-ferromagnetic order, while computational studies predict it to also exhibit a spontaneous polarization of 16 $\mu C/cm^2$ owing to an octahedral rotation induced improper mechanism. Using first principles density functional theory calculations, we investigate nine isostructural $AA'MnWO_6$ compounds through chemical substitution of alkali metal (A=Na, K, Rb) and rare earth cations (A'=La, Nd, Y), and find that the ferroelectric polarization can be enhanced by up to 150% by maximizing the difference in ionic size of the A and A' cations. We then identify the microscopic features responsible for this polarization through an examination of the tolerance factors, bond valences, and atomic displacement patterns. We anticipate that the crystal-chemistry criteria and analysis presented here can be extended to additional members of this family as well as guide the targeted design of novel multiferroics.

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