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First-principles investigation of anion ordering in $YBaFe_2O_5F$

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The introduction of a second anionic species to a perovskite is a promising way to modify its properties, but to realize the full potential of this approach it is desirable to control the ordering of the anion sublattice. We have studied the addition of fluorine to the cation- and vacancy-ordered perovskites $YBaFe_2O_5$ and $LaBaFe_2O_5$ as model systems to develop guidelines for achieving anion ordering. In addition to calculating the energy of different anion-ordered configurations, we have calculated the activation energy opposing the motion of fluorine out of the pre-existing anion vacancy sites. We find that factors such as octahedral tilt pattern, bond angle, bond length, and the choice of *A*-site cations affect the anion ordering, and some of these factors can be controlled using common experimental techniques to promote anion ordering.