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Density-functional study of the $\mathbf{Ba}_x\mathbf{Bi}_{(1-x)}(\mathbf{M}_{(1-x)/2})\mathbf{Ti}_{(1+x)/2}\mathbf{O}_3$ perovskite solid solution DENNIS JACKSON, Oregon State University, DAVID ROUNDY, Oregon State Univerity — Using density-functional theory we predict properties of the solid solution perovskites $Ba_xBi_{(1-x)}(M_{(1-x)/2})Ti_{(1+x)/2}O_3$ where M is Mg, Ni or Zn. These properties are strongly affected by the presence of both A-site and B-site disorder. We study all distinct orderings within a given $2 \times 2 \times 2$ supercell.

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