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Structure and Electronic Dependencies on Anion Order in Oxyfluoride Elpasolites[1] NENIAN CHARLES, Drexel University, JAMES RONDINELLI, Northwestern University — Complex oxyfluoride compounds are an emerging class of materials that aim to combine the advantageous properties of oxides and fluorides. Moreover, the ensuing order of the oxide and fluoride anions provides an additional knob to tune properties. However, there remains no complete set of design rules for realizing and controlling anion order in metal oxyfluorides. Here, we investigate the anion site order dependence on cation chemistry in the elpasolite double perovskite oxyfluoride family using group theoretical techniques and density functional theory (DFT) calculations. We enumerate hundreds of anion ordered structural variants with $A_2BMO_xF_{6-x}$ ($x = 1, 2, 3$) stoichiometry and develop a classification scheme based on characteristic symmetry adapted mode distortions exhibited within the family of compounds. Using DFT calculations we show that changing the d orbital filling of the M cation can modulate the relative stability among structural variants. Our results advance the understanding of anion order in oxyfluoride compounds and we anticipate that it will guide the synthetic stabilization of new oxyfluorides elpasolites.

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