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First Principles Design of A Heteroanionic Metal-Insulator Transition Compound LAUREN WALTERS, NATHAN SZYMANSKI, DANILO PUGGIONI, JAMES RONDINELLI, Northwestern University — Using symmetry principles and electronic structure calculations we designed a novel metal-insulator transition (MIT) compound MoON [1]. We draw parallels between MoON and the well-studied VO_2, demonstrating that properties such as the c/a lattice parameter ratio could be used for the design and identification of rutile MIT materials. The alpha and beta phase of MoON were identified from a set of prototype AB_2 structures based upon energetics, band gap, and the c/a ratio. We show that the heteroanionic *fac* ordering of the polyhedra are important for charge localization and singlet formation to open a band gap. Furthermore, our density functional calculations show how changes in the electronic band gap are driven by structural distortions, including 1D chain canting and dimer formation. Finally, we present design principles for the future prediction of metal-insulator transition materials. **Reference:** [1] N. Szymanski et al. Phys. Rev. Lett. **123**, 236402 (2019) **Funding Acknowledgement:** This work was supported by the National Science Foundation's (NSF) MRSEC program (DMR-1720139) at the Materials Research Center of Northwestern University. L. N.W. and J. M. R. were supported by NSF under DMR-1454688.

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