The 2022 Partnership for Research and Education in Materials

Use of Sr(B,B')O_3 Perovskites for transparent semiconductors

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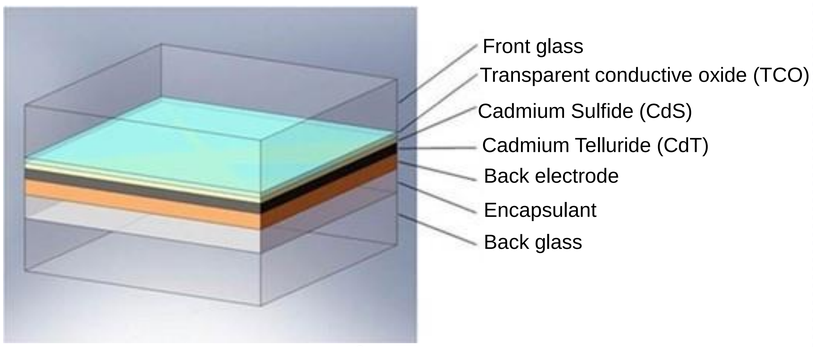
Transition toward solar technology

Efforts to mitigate climate change rely on a transition away from fossil fuels. Photovoltaics are a promising alternative. Solar cells require a transparent conductor (TC). The current state of the art material for this is indium tin oxide (ITO)

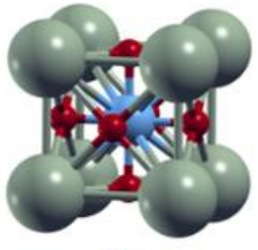


Anatomy of a photovoltaic cell [3]

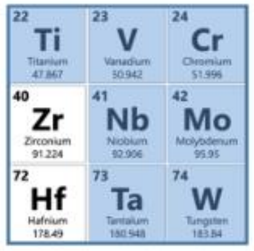
The logistical challenges of sourcing indium have motivated the search for alternative transparent conductors. One promising family[1] of transparent conducting materials is cubic Sr oxide perovskites.

Consideration of transparent perovskite semiconductors

Despite their attractive properties, no single perovskites shown below is both stable and a good transparent conductor. [2]



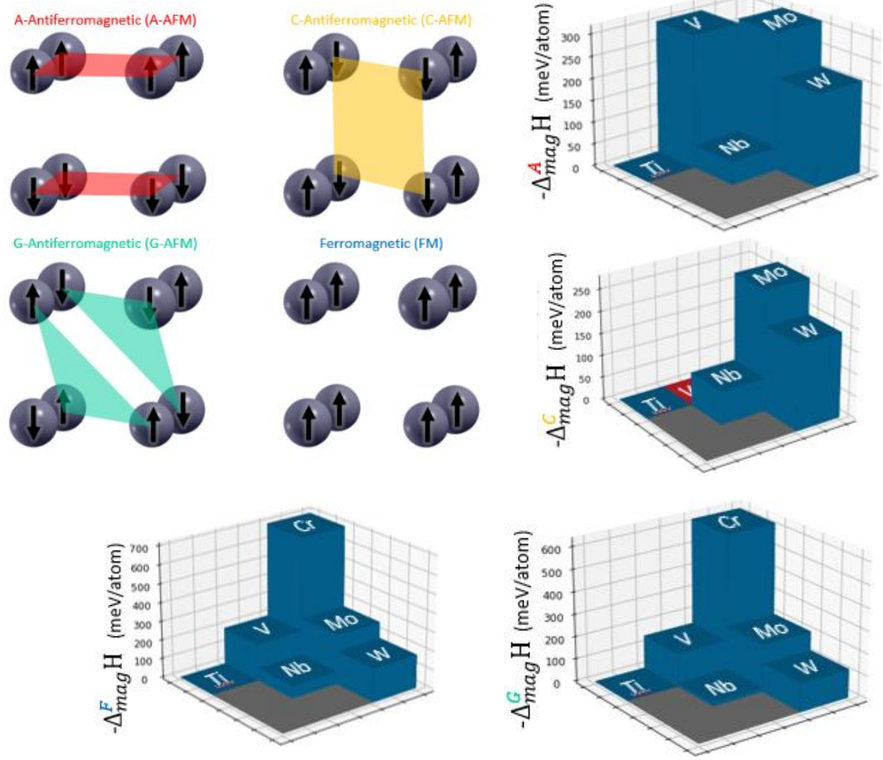
$SrBO_3$



High entropy perovskites show potential as stable TCs but their composition-processing- structure-property relations remain unstudied. DFT study of the single and double perovskites were carried out to elucidate these relations.

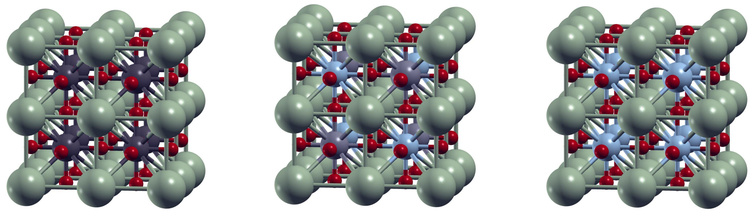
Enthalpies of magnetization of single perovskites

To understand the influence the magnetic ordering has on the structure of perovskites 4 different magnetic orderings will be taken into consideration, Ferromagnetic (FM), and 3 anti-ferromagnetic orderings (A, C, G). The enthalpies of each respective system were calculated.



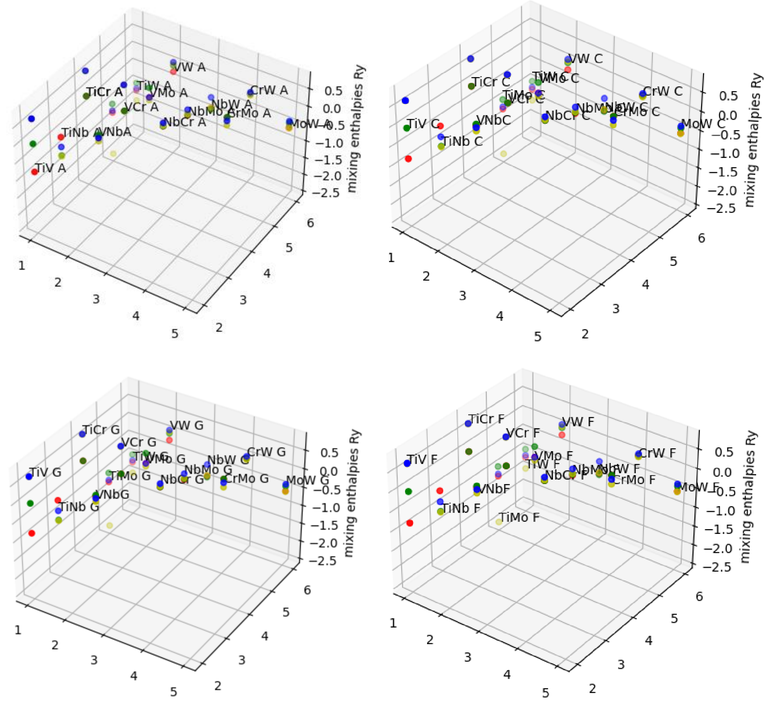
Data has yet to be collected for Chromium A-AFM, C-AFM, and Vanadium C-AFM

Based on the enthalpies of single and double perovskites the mixing enthalpies of the various cations were computed.



$SrBO_3$ $Sr(B,B')O_3$ $SrB'O_3$

Mixing enthalpies of Double Perovskites



Log plot of Mixing enthalpies in Ry

$$\Delta^{mag}_{mix}H(B,B') = H(B,B') - \frac{1}{2}[H(B,B) + H(B',B')]$$

Under FM and G-AFM ordering, the 3d transition metals are much more amenable to forming solid solutions. Engineering this magnetic ordering is predicted to stabilize these high entropy perovskites

References

[1] Rakesh A. Afre, et al. July 21, 2017. *Transparent Conducting Oxide Films For Various Applications: A Review*. Walchand Center for Research in Nanotechnology and Bionanotechnology.

[2] Lei Zhang, et al. December 14, 2015. *Correlated metals as transparent semi conductors*. Nature Materials

[3] . 2011. *Innovative Transition From Silicon Solar Cells To Thin Film*, m.energytrend.com

The Penn State REU program in Nanoscale Materials and Physics is supported by the Penn State Department of Physics and the Center for Nanoscale Science (NSF-MRSEC) and the National Science Foundation (DMR 2011839, and DMR 1851987).