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Computational Prediction and Characterization of M-X3-enes[1]
MICHAEL PUN[2], Bowdoin College and University of Florida, HENNIG MATERIALS THEORY LAB TEAM — Two dimensional (2D) materials are characterized as individual sheets of atomic thickness. In general, 2D materials are an exciting field of research because of the unique properties their structures present and the possible applications they promise. While the synthesis of 2D materials is crucial in order to realize applications for these materials, modeling of such materials is equally important to predict which materials are probable and thus worth pursuing. 2D materials can be modeled accurately using the computational quantum mechanical modeling method known as Density Functional Theory (DFT). This modeling can predict the formation energy of such 2D materials as well as several material properties and characteristics. Here we examine possible 2D materials of the form MX3 where M represents the 8 transition metals surrounding Zr in the periodic table and X includes the three chalcogens S, Se, and Te. 23 out of 27 of the materials examined are found to have formation energies below 200 meV/atom ranging from 44 meV/atom to 155 meV/atom. Those materials with formation energies below 200 meV/atom are characterized in terms of magnetic moment, Bader charge, band gap, and water solubility. Both direct and indirect band gap semiconductors are found as well as metals.

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