

Faces of Physics Presents:

## **Undergraduate Student to Doctoral Candidate: A Marshall Alumna's Perspective**

December 2<sup>nd</sup> at 7pm Eastern Time

<https://www.youtube.com/watch?v=2bORP16Kd18>



Emily Sutherland

### **Speaker's Biography:**

**Biography:** Emily Sutherland received her B.S. degree in 2019 from Marshall University where she double majored in physics, with an area of emphasis on applied physics, and applied mathematics. She was in the Marshall University Honors College, and served as President for the

school's chapter of the Society of Physics Students. She also worked as an undergraduate teaching assistant for the physics department and as a peer tutor. While at Marshall University she was inducted into the national honor societies for physics and for mathematics. Her capstone research projects were in the areas of theoretical solid state physics and numerical partial differential equations. Currently, she is a physics PhD candidate at Worcester Polytechnic Institute. Her dissertation research utilizes computational solid-state physics to model a family of 2D materials, known as MXenes, for applications in clean energy.

### **Talk Abstract:**

The journey through undergraduate work can be an intimidating one, especially for those interested in pursuing a doctorate. What classes should you take? What research should you do? How do you choose which PhD programs to apply to? What should you expect in grad school? Just how awful are the qualifying exams? I hope to offer insights on these questions from my own journey. This talk will first focus on my time at Marshall- classes, research, and extracurricular activities, and how they prepared me for graduate school. I will share my process of selecting and applying to PhD programs, and how I came to choose Worcester Polytechnic Institute. The focus will then shift to my experiences throughout the first two and a half years of my doctorate, including discussion of classwork, qualifiers, teaching, professional interactions, and choosing dissertation research. I will also discuss my current research.

### **A Density Functional Theory Study of Charge Transport in MXenes:**

Over the last decade, a new family of 2D materials known as MXenes have rapidly gained interest in the scientific community. Specifically in studies related to clean energy applications where 2D materials, such as graphene and transition-metal dichalcogenites, play a key role in the development of novel and sustainable devices. In general, MXenes have been found to be metallic with highly stable structures and excellent, tunable, charge transport properties. These properties make MXenes interesting candidates for use in energy storage, photovoltaics, photocatalysis, gas sensing, electrocatalysis, and more. My research uses Density Functional Theory (DFT) to study the charge transport properties of MXenes. DFT is based on quantum mechanics, and is one of the most popular methods used for solid-state physics and materials science simulations. The method approximates ground state properties of a many-electron system in terms of its electron density function. This allows us to make accurate predictions of structural, electronic, and optical properties for many MXenes. Our current focus is quantifying and identifying trends in the tunability of electronic properties, such as density of states and work function, by adjusting MXene composition or allowing surface adsorption of other molecules.