**MXene Synthesis in silico**

Susan B. Sinnott, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16801, USA

A driving force for research is the discovery and design of new materials to improve existing technologies or enable new applications. Material modeling methods are now widely applied in pursuit of this objective. This presentation will review the evolution of some common material modeling methods and their integration with cutting-edge experimental techniques. Illustrative applications will be discussed within the context of layered or two-dimensional materials and will include exploration of their use in specific applications. The presentation will conclude with a discussion of the future outlook of materials modeling within the context of material design and discovery.