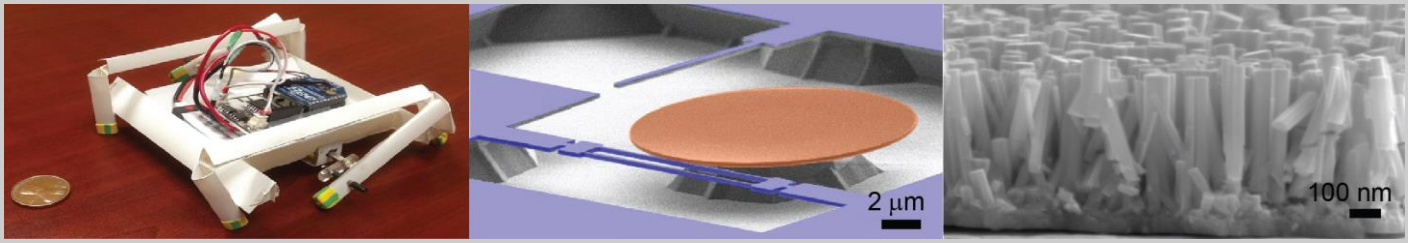
WPI MECHANICAL ENGINEERING



WPI ME Graduate Seminar Series 2019-2020

Application of Computational Thermodynamics in Solid Oxide Fuel Cells

Yu Zhong, Ph.D.
Associate Professor, Mechanical Engineering
Worcester Polytechnic Institute

10:00-10:50 am, Wednesday, March 4
Higgins Labs 218

High sintering and operation temperatures promote unwanted interface reactions in Solid Oxide Fuel Cell (SOFC), especially at the cathode-air-electrolyte triple phase boundary (TPB). The composition changes and phase stability at TPB have been identified as the dominant mechanism for long-term degradation, which is a critical parameter for SOFC. It is greatly needed to use the computational thermodynamics (CALPHAD) approach to investigate the phase equilibria between the cathode (perovskite) and the electrolyte (doped zirconia).

The talk will cover our recent discoveries on the following topics: 1.) the TPB phase stabilities (formation of LZO and SZO); 2.) the quantitative defect chemistry analysis for perovskite; 3.) the electrical property prediction (electronic and ionic conductivity) for perovskite and zirconia; 4.) the thermomechanical properties for perovskite (CTE mismatch, chemical expansion); 5.) the reactions between cathode and gas impurities, including CO2, SO2, H2O, and Cr.

Meanwhile, several other examples of using our unique Integrated Materials and Processes Design (IMPD) approach in alloys and ceramics will be briefly covered.

About the Speaker

Dr. Yu Zhong is currently an Associate Professor in Mechanical Engineering at Worcester Polytechnic Institute (WPI). He received his Ph.D. from Penn State University (2005). After a short-term working as Research Associate, he joined Saint-Gobain High-Performance Materials Research Center in Northborough, MA. He had built up his career there as an internal technical consultant focusing on the application of thermodynamics and kinetics to various R&D projects. In 2013, He moved to Florida International University (FIU) as Assistant Professor and joined WPI in 2017. Dr. Zhong received the TMS FMD Young Leaders Professional Development Award in 2016 and ONR summer faculty fellowship in 2015, 2016, and 2017. He has more than 49 peer-reviewed journal papers published/accepted, 2 book chapters, and 2 patents. His research is currently supported by the Department of Energy (DOE), National Science Foundation (NSF), American Chemical Society (ACS), and Advance Casting Research Center (ACRC).