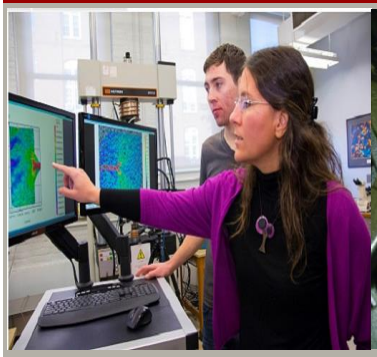
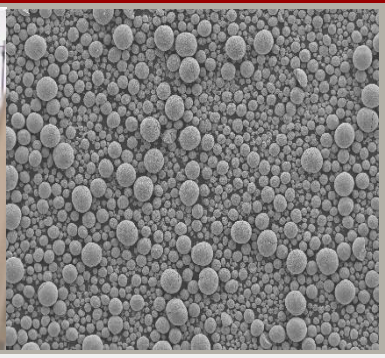
WPI

Materials Science & Engineering



Wednesday September 12, 2018
12pm

Washburn shop #229

Prof. Yu Zhong
Associate Professor
Mechanical Engineering

MTE Seminar Series

Application of Computational Thermodynamics in Solid Oxide Fuel Cell

Abstract:

(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 the 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.