… THE NEW DEAL
FOR THE
NANO WORLD ….

Department of Industrial Engineering

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Operando Spectroscopy of polymer electrolyte/catalyst interfaces

Theory and experimental vibrational spectroscopy of catalyst/electrolyte interfaces.
The lectures will cover the structure of proton exchange membranes (PEMs), their applications in PEM reactors for power generation and chemical transformations, and the analyses of operando spectra of PEM based membrane electrode assemblies.
The analyses of PEM/catalyst interfaces require the use of density functional theory based normal mode analyses and visualization of vibrational mode eigenvectors. Basic considerations in the design of operando cells and corresponding membrane electrode assemblies will be discussed. The use of density functional theory calculations for normal mode analysis and electron density topological analysis (QTAIM) will introduced. Several case studies will be discussed.
Total lecture time: 12 hours over 2 weeks.
Week 1 topics:
a. PEM structures and function.
b. Incorporation of PEM/catalyst interfaces into electrochemical reactors.
c. Modification of practical reactors for operando spectroscopy
d. Raman and IR spectroscopy of PEMs and PEM/catalyst interfaces
Week 2 topics
a. Correlation of hydration dependent IR spectroscopy to proton transport mechanisms.
b. Density functional theory normal mode analysis and visualization of eigenvector animations.
c. Examination of gradients and Laplacians of electron densities for bond critical points of PEMs and PEM/catalyst interfaces.