Improved Catalysts for the Hydrogen Economy

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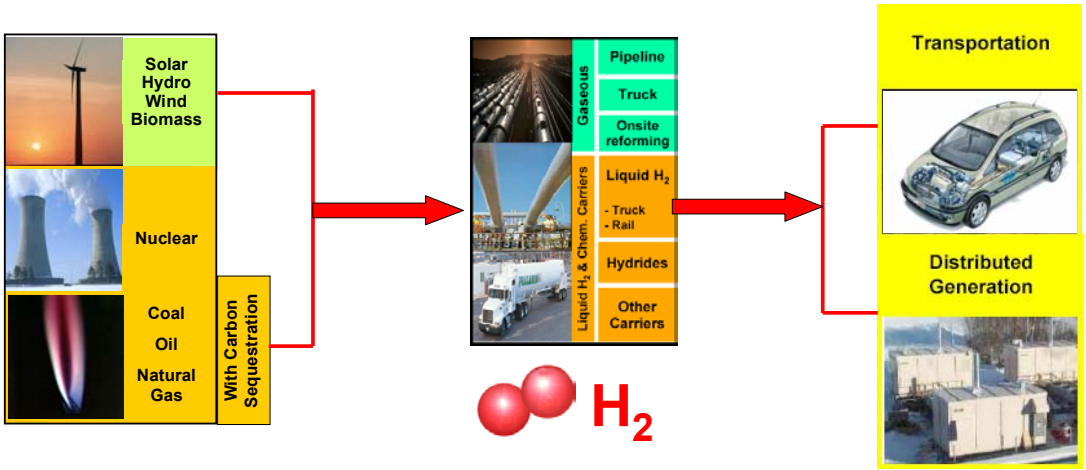
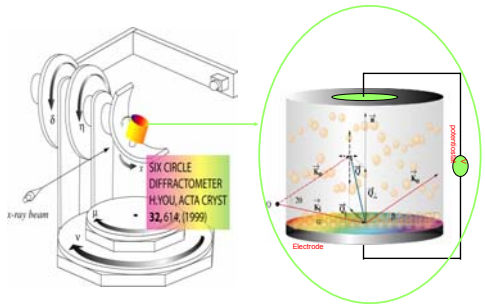


Catalysis is a crosscutting issue in development of a hydrogen economy

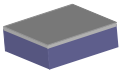
- **Improved catalysts with lower cost and improved efficiency are needed for fuel cells, storage, and production**
- **Fundamental understanding of molecular level processes needed to find new catalysts**
- **Requires detailed characterization of catalytic sites and interaction of reactants with them under realistic conditions such as for oxygen reduction at a Pt cathode (see below)**

X-ray Studies at ANL Advanced Photon Source

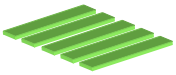


X-ray/electrochemistry cell to investigate oxygen reduction reactants and intermediates

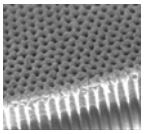
Pt catalyst surfaces with increasing complexity

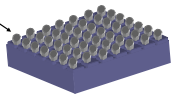


flat Pt surface

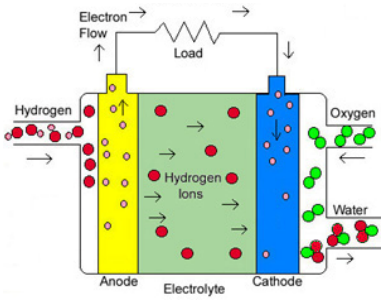


stepped Pt surface



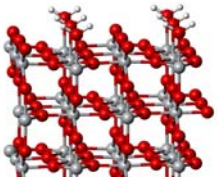


Simulation and Modeling

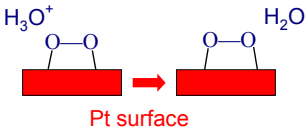


Develop realistic models of oxygen reduction mechanisms on Pt catalysts

Study effect of solvent, electric fields, and use of Pt-X alloys on reaction mechanisms



Structure of adsorbed species at the electrolyte/cathode interface, e.g. water on RuO_2 (110) surface



Potential energy surface of electrocatalytic reactions, e.g, $PtO_2(ads) + H^+(aq) + e^- \rightarrow PtOOH$

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