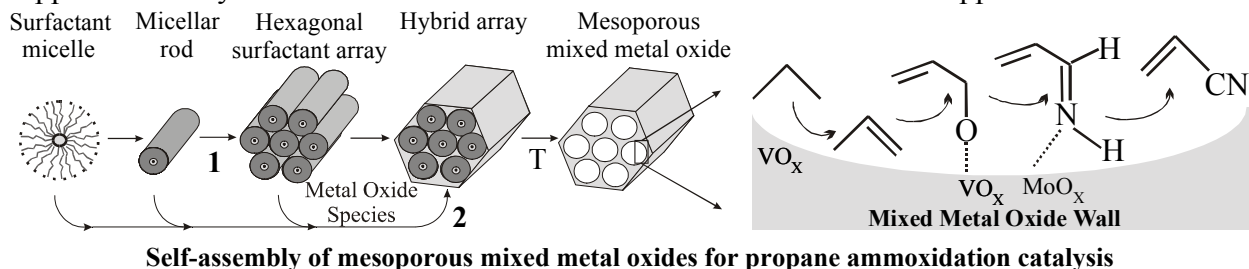


CAREER: Ordered Mesoporous Mixed Metal Oxides: An Integrated Research and Education Program

This career development plan seeks to introduce the concept of molecular engineering of complicated mesoporous materials in both research and chemical engineering education. In research, this proposal aims at developing comprehensive methods of design of mesoporous multicomponent V-Mo-M-O (M= Nb, Te, Sb, etc.) oxides and elucidating the fundamental relationships between the molecular structure and catalytic function of these well-defined model mixed metal oxide systems. The targeted application of these model catalysts is in selective ammoxidation of propane to acrylonitrile, which an important chemical intermediate. The specific research and education objectives of the five-year career development plan are:

- **Developing synthesis methods for model mesoporous V-Mo-M-O mixed metal oxides**
- **Establishing the bulk and surface molecular structure-reactivity/selectivity relationships for propane ammoxidation to acrylonitrile over model mesoporous V-Mo-M-O metal oxides**
- **Integrating molecular engineering into traditional chemical engineering education**

Model mesoporous V-Mo-M-O oxides will be synthesized via two novel self-assembly approaches employing molecular and nanocrystalline building blocks in the presence of mesoscale supramolecular surfactant arrays and block copolymers. Various surface chemical probes will be employed to elucidate the nature, number, structure and specific activity of surface redox, acidic and basic sites present in these model mixed metal oxide catalysts. Additional fundamental insights will come from parallel molecular modeling studies of structure and reactivity of surface VO_x , MoO_x , NbO_x , SbO_x and TeO_x species. The molecular structure-reactivity/selectivity relationships from this research program will be used to assist in the design of improved catalysts and the development of fundamental mechanistic models for alkane ammoxidation over mixed metal oxide catalysts. This proposed research also involves international and industrial collaborations. Unique expertise exists at Cincinnati for this proposed research. The PI adds considerable experience in the area of catalytic mixed metal oxides to on-going advanced materials research at the University of Cincinnati. The PI's current research efforts in functional porous inorganic materials have already secured NSF, state, industrial, and university support. Recently established industrial collaborations have also created opportunities for



technology transfer to the US chemical industry, which is already under way.

The proposed education program is aimed at integrating molecular engineering of advanced materials into traditional chemical engineering education and training chemical engineers with a strong background in molecular engineering of chemical and biological systems. The *broader impacts* of the proposed educational activities include developing two courses on molecular engineering for undergraduate and graduate students, implementing a molecular engineering research program for undergraduates, and the outreach to underrepresented groups. Two new quarter-based courses on *Molecular Engineering of Advanced Materials* and *Interfacial and Surface Phenomena* will be developed and offered to chemical engineering students. The molecular engineering research program will consist of funded undergraduate participation in molecular engineering research and project design related to applications of advanced materials. The outreach efforts will be directed towards improving higher education opportunities for minority and women engineers by alerting them to the graduate research opportunities in molecular engineering at the University of Cincinnati. The proposed educational activities will promote interest of chemical engineering students in molecular engineering and enhance their awareness of the impact of advanced materials on the chemical processing industry. These educational activities have already resulted in a course redesign of *Computational Chemistry for Engineers*, organization of AIChE, ACS, and local meetings on heterogeneous catalysis and advanced materials by the PI, and the recruitment of minority and women students.