Materials Chemistry

Description: Scattering techniques (using spallation and steady-state neutron and synchrotron x-ray sources) are combined with thermodynamic, scanning probe and computer simulation methods to develop a comprehensive understanding of the structure and dynamics of molecular films adsorbed on surfaces and within porous media. These studies are important because they provide the necessary information for developing quantitative theoretical descriptions of molecule-molecule and molecule-surface interactions. Elastic and high-resolution inelastic neutron scattering methods are used to monitor changes in the structure and dynamics associated with phase transformations. The goal of this program is to initiate and advance methods for investigating the microscopic properties associated with novel two- and three-dimensional materials, some of which may be chemically active. Recently, these experimental methods have been used to probe the changes in the physical and chemical properties of simple molecules adsorbed on uniquely prepared nanoparticles of MgO and doped metal oxide powders. This work is aimed at identifying how the interfacial region of materials mediates simple chemical reactions by investigating the interplay between chemical activity and changes in microscopic structural and dynamical properties of the system. Finally, efforts continue to design, develop and construct state-of-the-art scientific devices geared toward the implementation of elastic and inelastic neutron and x-ray scattering investigations at major facilities.

Program Highlights:

Investigated the wetting properties of adsorbed atomic (At, Xe) and molecular(NH3, Sn(CH3)4 films using a combination of neutron diffraction , adsorption isotherms and computer simulations.

Characterized the rotational tunneling properties of thin films of methane on Mao(100) surfaces which illustrate the cross over from 2D-to-3D.

Developed a novel (potentially patentable) process for producing pure and doped metal oxides of the form MxRlxO (where M= Mg, Zn and R= Ag, Au, Cr, Cu, Zn, Li, Ni).

Employed X-ray image plate technology to investigate the structural properties of atomic and molecular films adsorbed on BN and MgO surfaces.

Developed a fully automated, Labview based, adsorption isotherm apparatus for use in studying adsorbed films and for characterizing porous media which may be chemically active.

Impact

The combination of diffraction and adsorption isotherm techniques has led to the development of a microscopic description of the thermodynamic signatures. Stimulated a collaboration with BOC whose interests are in using these techniques for understanding 'gas separation processes.

Our inelastic measurements of the tunneling properties of methane on MgO serves as a prototype for developing realistic interaction potentials for adsorption on MgO.

The pure and doped MgO powders synthesized to date have shown chemical activity one-to-two orders of magnitude greater than commercially available powders for catalyzing, the decomposition of N,O.

Interactions: Collaborations are maintained with investigators throughout the U.S. and Europe; University of Missouri (J.M. Phillips (UMKC), H.Taub (UMQ, Wesleyan University (R. J. Rollefson), Lafayette College (A. Novaco), and Rutherford-Appleton Lab (C. Carlisle and D. Martin (ISIS)), University of Kiel, Germany (W. Press and B. Asmussen), BNL (L. Passell (Physics)) and Y. Zhu (DAS)), Warner-Lambert (Y. Zhu, W. Vreeland (Schick Razor)). Catalysis and Interfacial Chemistry Effort (CICE) (BNL *Photoinduced Molecular Dynamics in Gas and Condensed* Phases (White) and *Catalysis: Reactivity and Structure* (Hrbek)).

Personnel: J. Z. Larese (BNL, PI), W. Kunnmann **(BNL, synthesis), D. Johnson (BNL, RA),** Deepak Poondi (BNL, RA), Andrea Frietaa (BNL, RA), Micheal Sprung (Kiel Univ., Graduate Student).

Recognition: 8 Invited talks FY97-FY98, PI for *HERMES 1*, a high resolution crystal backscattering spectrometer at LANSCE, Patent preparation for synthesis of pure and doped Mgo powders, Invited reviews (Current Opinion in Solid State & Materials Science and Surface Science Reports), Member ISIS Spallation Neutron Source Experimental Review/Scheduling Panel, External examiner for Stuart Campbell Phl). Defense, Salford Univ. England. Spokesperson NSLS Beamline X713. Adjunct Professor, Wesleyan University

Budget :$495K