

Final Report

***Thermodynamic and X-ray Studies of Electrically-Ordered Adsorbed
Phases***

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Project Abstract

This project was a collaborative effort between Dr Teresa Burns and Dr John Larese to study the physisorption of polar molecules on ionic substrates. The work will be completed at both Coastal Carolina University and Brookhaven National Laboratory. The goals of the research are: 1) to provide detailed thermodynamic information about dipolar molecules adsorbed on ionic substrates, critical to accurately modeling the systems of interest using a spin-1 Ising model; 2) to study the structure of the adsorbed layer from the gas phase, experimentally verifying the application of the model to these systems; 3) to extend the modeling studies and structural measurements to systems adsorbed from the liquid phase. The systems will be studied using thermodynamic techniques, e.g., adsorption isotherm both from the gas and liquid phase, and x-ray structural measurements. This project will strengthen the physical science research efforts at CCU, and hence in South Carolina.

Project Summary

The funding of this proposal started July 2001. During Summers 2002, 2003, and 2004, PI Burns traveled to the University of Tennessee to work with Dr John Larese, to perform thermodynamic measurements of halogenated methanes adsorbed on MgO. Two systems were studied in detail, methyl bromide and methyl iodine. The methyl bromide system is almost completely characterized. Incomplete wetting is observed both above and below the 3D triple point temperature, with two layers forming before bulk condensation. The 2D compressibility for the first and second layer was calculated, and the isosteric heat of adsorption will be calculated. The results are expected to be ready for submission for publication shortly.

Some of this work was completed with student TJ Harper during Summer 2002. Mr. Harper presented preliminary results at the 2003 APS March Meeting in Austin, TX, and the South Carolina Academy of Sciences Meeting at Clemson University, March 2003. Note that Mr Harper, after spending the summer doing research supported by this grant, decided to pursue a graduate degree in chemistry. He has subsequently completed a master's degree and works for a small company that searches for natural product pharmaceuticals. Additional presentations are listed below.

On campus at CCU, we have built a gas handling system to do the same kinds of measurements here. Undergraduate students have developed the LabView code that control the automated gas handling system built at Coastal, and have rebuilt the hardware based on the lessons learned from Dr Larese's lab. Joseph Benckert presented his work at the Coastal Carolina University Undergraduate Research Symposium in May 2002; he won honorable mention for his work. He is currently pursuing a graduate degree in Physics at North Carolina University. Undergraduates Ipshita Chakraborty, and Roy Taylor also contributed to this work.

A second focus of the grant is to develop materials and methods for the study of molecules adsorbed from solution. The systems iodomethane and Triton X on activated carbon and graphite were studied, mainly to establish measurement methods. Additionally, we studied adsorption of benzene on graphite. This system was chosen for two reasons: it is of interest because of the match between the ring structure of the adsorbate and the substrate and because it could be studied in parallel to UV-VIS detection with a resonance enhanced multi-photon ionization (REMPI) system developed at CCU by Dr. John Reddic in the Chemistry Department. The adsorbate concentration change could be measured by detecting the REMPI signal change in the head-space gas above the sample. It is therefore unnecessary to physically separate the supernatant from the sample, and allows almost *in situ* monitoring of the concentration change of the adsorbate. These studies were performed by undergraduate student Katherine Cilwa; she presented her work at the Southern Atlantic Coast Section of the American Association of Physics Teachers meeting at Coastal Carolina University, in March 2003. She also entered graduate school to study physical chemistry at the Ohio State University. Undergraduates Trent Bostic and Charles Molnar also contributed to this work.

The research outcomes of this grant were impacted by Dr John Larese's shift from Brookhaven National Laboratory to University of Tennessee. However, the associated outcomes have been significant. The grant supported seven undergraduates in research efforts. Of the seven, six pursued additional studies in the sciences. Two of the seven have been women. Since CCU is not a research institute, and our primary mission is teaching, this grant has been successful in helping the institution meet that goal.

Undergraduate Students Supported:

Joseph Benckert

Trent Bostic

Ipshita Chakraborty

Katherine Cilwa

TJ Harper

Charles Molnar

Roy Taylor

Travel Supported:

Teresa Burns, TJ Harper, Summer 2002, in residence at University of Tennessee to perform isotherm studies of methyl bromide on MgO.

Teresa Burns, TJ Harper, Summer 2003, 2004, in residence at University of Tennessee to perform isotherm studies of methyl bromide on MgO.

Teresa Burns, TJ Harper, Austin, TX, to attend the 2003 APS March Meeting, and to present outcomes of research.

Teresa Burns, TJ Harper, Clemson, SC, March 2003, South Carolina Academy of Sciences Meeting to present outcomes of research.

Teresa Burns, TJ Harper, Los Angeles, CA, to attend the 2004 APS March Meeting, and to present outcomes of research.

Presentations:

Joseph Benckert, Teresa Burns, *Control of Gas Handling System Using LabVIEW*, Coastal Carolina University Undergraduate Research Symposium, May 2002; he won honorable mention for his work.

TJ Harper, TE Burns, JZ Larese, *Adsorption Isotherm Studies of Methyl Bromide on MgO*, 2003 APS March Meeting in Austin, TX, March 2003.

TJ Harper, TE Burns, JZ Larese, *Adsorption Isotherm Studies of Methyl Bromide on MgO*, South Carolina Academy of Sciences Meeting at Clemson University, March 2003.

K Cilwa, TE Burns, *Materials and Methods for Benzene Adsorption on Activated Carbon*, Southern Atlantic Coast Section of the American Association of Physics Teachers meeting at Coastal Carolina University, March 2003.

TE Burns, JZ Larese, *Adsorption Isotherm Studies of Halogenated Methanes on Magnesium Oxide*, American Physical Society Meeting, Los Angeles, CA, March 2005

Equipment Purchased:

Quantachrome Nova 2200 Surface Adsorption System

National Instruments DAQ Board, Shielded terminal block and LabVIEW software

Laptop computer

Neocera Temperature controller

Various vacuum components and valve upgrades

Gases and liquid nitrogen in support of research efforts