

M.W. Roth, E. Maldonado, University of Northern Iowa  
L. Firlej, LCVN, Universit Montpellier  
B. Kuchta, Laboratoire Chimie Provence, Universit de Provence,  
Carlos Wexler, University of Missouri Department of Physics and Astronomy

### **Computer simulations of tetracosane (C<sub>24</sub>H<sub>50</sub>) bilayers deposited onto graphite**

A collaboration involving a UNI undergraduate as well as faculty in France has resulted in computer simulations of long molecules on surfaces - tetracosane (C<sub>24</sub>H<sub>50</sub>) bilayers deposited on a graphite substrate - in the temperature range  $100 \text{ K} \leq T \leq 450 \text{ K}$ . Both layers exhibit strong coupling between the internal molecular degrees of freedom and bulk behavior but because of the different boundary conditions between layers, they exhibit distinctly different dynamics and phase transition signatures. Structural, thermodynamic and bond - orientational distributions and parameters are utilized in understanding the solid, intermediate and liquid phases presented in and phase transitions presented by the system.