

# Physics Colloquium

Michigan Technological University

Thursday, October 11, 2007

4:00 pm

Room 139, Fisher Hall

## Self-Assembly of Organic Adsorbates on Metal and Semiconductor Surfaces.

**Frank Hagelberg**

Department of Physics, Astronomy, and Geology

East Tennessee State University

Johnson City, TN 37614

**Abstract:** Self-assembled monolayers (SAMs) are molecular films that form spontaneously on solid surfaces. Numerous applications in tribology, chemical and biological sensing, optics, and nanotechnology have been identified for these systems. Among the many varieties of SAMs, alkanethiol molecules on the Au(111) surface have been given special attention because of the relative simplicity of their structure, their highly stable and ordered SAM patterns, and the ease of preparing the Au(111) surface. Despite the elementary nature of this system, its observation in various experiments has led to controversial results. Key issues in this debate are the stability of the thiol S – H head group on the gold surface and the dimerization behavior of the adsorbates. These problems have been addressed by Density Functional Theory computations for the case of methanethiol, resulting in a new unified model<sup>1</sup> of SAM formation on gold surfaces that is consistent with all related experimental observations. Specifically, it was found that the S-H bond of the adsorbate remains intact when the methanethiol molecules are adsorbed on the regular Au(111) surface. It breaks, however, when admission is made for surface defects. It was further demonstrated that methanethiol adsorbates on Au(111) organize in dimers. For methylthiolate, it was shown that dimerization exists below a certain coverage threshold and is absent at high coverage levels, in full agreement with experimental data. In addition to thiol attached to gold, monolayers formed by propanol-1 on the Si(001) surface will be highlighted in this presentation, providing an example for a dissociative reaction between an organic adsorbate and a reconstructed semiconductor substrate.

[1] J.-G. Zhou, F.Hagelberg, Phys.Rev.Lett. 97, 45505 (2006).

**Biography-** Frank Hagelberg received his Ph.D. from the University of Bonn, Germany in 1989. From 1990-92, he was a Feodor Lynen Fellow of the Alexander von Humbolt Foundation. He was a Visiting Associate Professor at the State University of New York at Albany from 1992-1996. Subsequently, he joined the Physics Department of Jackson State University as an Assistant Professor. He was promoted to Associate Professor in 2002, and then to Professor in 2007. He moved to East Tennessee State University in 2007. He has been cited in the “Who’s who among America’s teachers” in 2000. His research interest includes theoretical and computational analysis of atomic and molecular clusters, surfaces and interfaces, molecular reactions under endothermic conditions; non-adiabatic Quantum Dynamics of small molecular species. He is well known in molecular electronics community for his pioneering work on Self-assembled monolayer on Au substrate.