

UNH Materials Science Seminar

11:10-12:00, Thursday, April 21, 2005

DeMeritt Hall 209B

University of New Hampshire

Free and Deposited Silicon Based Clusters: A Computational Study

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Extensive experimental and theoretical investigations have focused on the size evolution of pure silicon clusters. Recently, silicon clusters with atomic impurities have attracted substantial interest as the microscopic counterparts of doped Silicon crystals or surfaces which are used abundantly in electronic materials. Four years ago, the first experimental evidence was given for the existence of endohedral Silicon clusters of the form $TM@Si_N$ where TM stands for a transition metal atom. This presentation will include an interpretation of these newly detected species in terms of geometry, stability and bonding properties. Size evolution features characteristic of Metal – Silicon clusters will be discussed by the examples of $CuSi_N$ and WSi_N with $N \leq 12$. The talk will further address the architectural features of Polyhedral Oligomeric Silsesquioxane (POSS) cages and highlight their capacity to encapsulate foreign alkali metal as well as halogen atoms. Also, recent work on deposited silicon clusters will be discussed.

Frank Hagelberg is an Associate Professor of Physics at the Center for Molecular Structure and Interactions, Jackson State University. He completed his Ph.D. in 1989 at the University of Bonn, Germany, in the field of experimental nuclear physics and was converted into a theorist during his subsequent stay at the State University of New York at Albany as a Feodor Lynen Fellow of the Alexander von Humboldt Foundation. His current research focuses on the theory of finite systems, in particular clusters in the gas phase or attached to substrates, as well as molecular quantum dynamics.