

T_CSUH Special Seminar

Texas Center for Superconductivity at the University of Houston



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Norfolk, Virginia

“Structural Kinetics, Electronic and Optical Properties of Organic Molecules Adsorbed on Solid Surfaces”

Friday, January 12, 2007

Room 102, University of Houston Science Center
2:00 p.m. – 3:00 p.m.

Abstract

Structural kinetics of molecular aggregates and adsorption of organic molecules on metallic and semiconductor surfaces are studied by first principle methods within Density Functional Theory (DFT). Equilibrium geometries of molecular aggregates and molecules adsorbed on solid surfaces are determined through the total energy minimization method. Electron energy structure and optical functions of solid surfaces and effects of the adsorption of organic molecules are studied by first principle evaluation of eigen-value and eigen-vector problems using ab initio pseudopotentials (PP). Intermolecular interaction is shown to be responsible for substantial modifications of optical spectra of molecular aggregates. It is demonstrated that adsorption of water on transition metal surfaces (silver, gold) could be monitored through differential linear optics (e.g. differential reflectance anisotropy). Electronic structure and optical properties of complex organic dye molecules (Rhodamine 6G) strongly depends on the molecular aggregation. Predicted electron energy structure modifications of silicon surfaces due to the adsorption of ethanol explain observed enhancement of sum frequency generation intensity from nanostructured silicon. Theoretical results are discussed in comparison with optical spectroscopy data (luminescence, optical absorption, reflectance, etc).

Bio

Dr. Vladimir I. Gavrilenko is an Associate Research Professor in the Center of Materials Research at Norfolk State University. He obtained his Ph.D. in 1979 and D.Sc in 1990 from the National Academy of Science of Ukraine. He is working in the field of computational materials science, including first principle studies of equilibrium atomic geometries, structural transformations, linear and non-linear optical properties of different solid and soft condensed materials, and physics and chemistry on surfaces and interfaces. He is an author or co-author of more than 100 scientific publications, including two books and a patent. He is member of APS (life member) and OSA, and he has served as a member of organizing committees of several domestic and international conferences and meetings.

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