

# T<sub>c</sub>SUH Special Seminar

Texas Center for Superconductivity at the University of Houston

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### “Optical Properties of Semiconductor Surfaces and Interfaces: First Principle Study”

**Monday, December 12, 2005**

Room 102, University of Houston Science Center  
12:00 noon – 1:00 p.m.

#### Abstract

Electron energy structure and linear and non-linear optical properties of group III-nitride compounds, as well as group IV semiconductors (bulk, surfaces, and interfaces) are studied by first principle evaluation of eigen-value and eigen-vector problems using full potential linearized augmented plane wave (FLAPW) and *ab initio* pseudopotentials (PP) approaches. Equilibrium surface/interface geometries are determined through the total energy minimization method. Optical responses from solid surfaces and effects of the adsorption of inorganic elements and organic molecules are studied. Intermolecular interaction is shown to be responsible for substantial modifications of optical spectra of molecular aggregates. Predictions of second harmonic generation (SHG) from semiconductor surfaces and interfaces are discussed. Effects of rehybridization of atomic bonds and electric field induced second harmonic (EFISH) response are considered. Strong contributions to the SHG efficiency of electron excitations from surface atom orbitals are demonstrated for Si(001) and GaN(0001) surfaces and the Ge/Si(001) interface. Adsorption of Ga on the N-terminated GaN(0001) surface results in a substantial evolution of the surface related SHG features. The predicted spectroscopic results from semiconductor surfaces and interfaces are discussed in comparison with experiment.

#### Bio

Dr. Vladimir I. Gavrilenko is an associate research professor at the Center of Materials Research at Norfolk State University, Norfolk, Virginia. He obtained his PhD 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, is a member of APS (life member) and Optical Society of America (OSA), and has served as a member of organizing committees of several domestic and international conferences and meetings.

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