Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

**Optical Properties of Rhodamine 6G Laser Dye and Ag-Nanoparticle Aggregates** M.A. NOGINOV, M. VONDROVA, S.M. WILLIAMS, M. BAHOURA, V.I. GAVRILENKO, S.M. BLACK, A. SYKES, Center for Materials Research, Norfolk State University, Norfolk, VA, V.P. DRACHEV, V.M. SHALAEV, Purdue University, West Lafayette, IN — Optical absorption and luminescence spectra of Rhodamine 6G (Rh6G) laser dye of different concentration with a solution of aggregated silver nanoparticles are studied. New emission band located near 610 nm is found at very high concentration of Rh6G and/or in a solution of Rh6G and Ag nanoparticles. Electron energy structure and optical functions of single Rh6G molecules, molecular complexes, and Rh6G molecules adsorbed on Ag(111) surface are studied by generalized gradient approximation method within density functional theory using *ab initio* pseudopotentials. Equilibrium geometries of the systems studied are obtained from both molecular dynamics simulations and X-ray diffraction measurements. Electronic structure of J-type molecular complexes (when two molecules aligned along their dipole moment axes) substantially differs from that of H-type aggregates (with parallel and anti-parallel molecular dipole moments). It is demonstrated that new luminescence line is associated with J-type molecular complexes. Observed modifications of optical properties of Rh6G and Rh6G+Ag complexes are explained in terms of both the changes of electronic structure of the systems and due to the electromagnetic interactions of dipole-dipole and dipole-surface types.

Vladimir Gavrilenko
Center for MAterials Research, Norfolk State University, Norfolk VA 23504

Date submitted: 01 Dec 2004 Electronic form version 1.4