Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Optical properties of the Folic Acid/APTMS/TiO_2 nanosystems[1]

VOLODYMYR TURKOWSKI, MICHAEL LEUENBERGER, TALAT RAHMAN, DUY LE, Dept. of Physics and NSTC, Univ. of Central Florida, Orlando, FL 32816, SUDIPTA SEAL, AMPAC, Univ. of Central Florida, Orlando, FL 32816, SANKU MALLIK, Dept. of Pharmaceutical Sciences, North Dakota State Univ., Fargo, ND 58105, ANDRE GESQUIERE, NSTC, Univ. of Central Florida, Orlando, FL 32816

— Our photoluminescence experiments on folic acid (FA) conjugated nanoparticles of TiO_2, CeO_2 and SiO_2 show great promise for a variety of optoelectronic applications for these materials, in particular in the field of modern molecular photoelectronic devices, since they demonstrate a dramatic increase of the photoemission intensity at wavelengths between 500 to 700 nm when the nanoparticles are coated with the 3-aminopropyltrimethoxylane (APTMS) linker/spacer molecule. We report here results of accompanying time-dependent density- functional theory studies of the FA/APTMS/TiO_2 nanosystems by using the B3LYP exchange-correlation potential. We demonstrate that the large increase of the photoemission is due to enhanced optical transitions which involve the intermediate energy levels related to the APTMS states. We present details of the geometric and electronic structure and excited states of our nanosystems and their dependence on the characteristics of the nanoparticle. We discuss possible optoelectronic applications for this effect.

[1]Work supported in part by DOE-DE-FG02-07ER15842.

Volodymyr Turkowski
Dept. of Physics and NSTC, Univ. of Central Florida, Orlando, FL 32816

Date submitted: 29 Nov 2008 Electronic form version 1.4