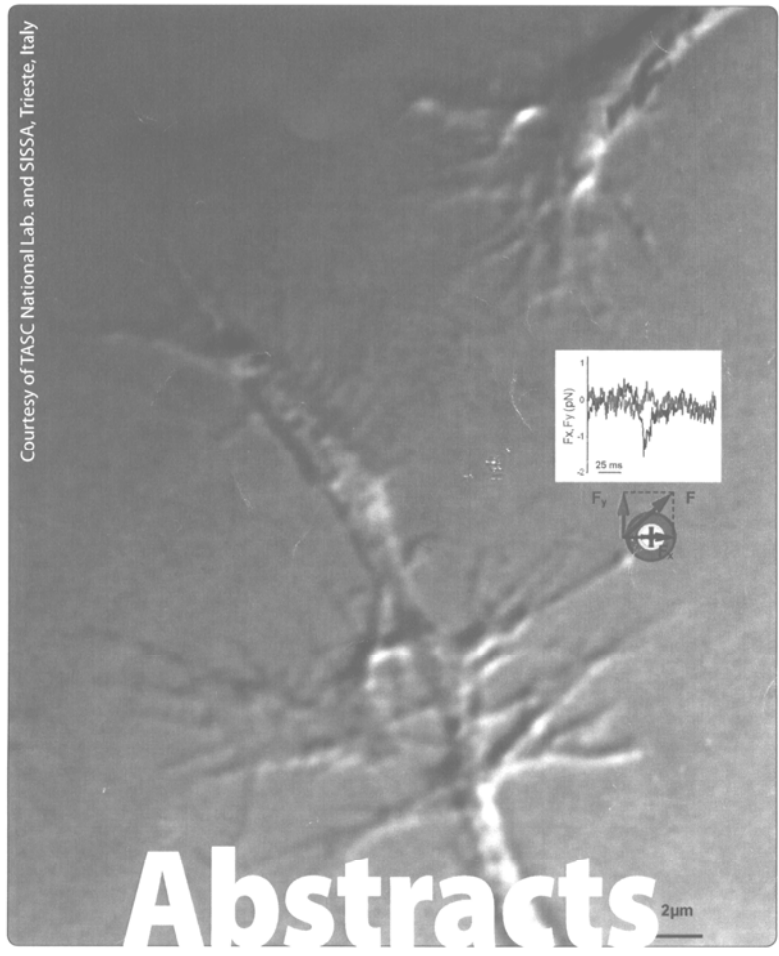


Workshop on

Trends in nanoscience: theory, experiment, technology



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analytical solutions are available for comparison. The other GNP shapes include nanorods and nanoprisms, tuning their plasmon modes across the whole visible and near infrared range. The theoretical spectra will be compared with experimental data from synthesized samples in our laboratory. The aim is to explain and better understand how the layers of cetyltrimethyl ammonium bromide (CTAB) surfactant, methoxy polyethylene glycol-thiol (mPEG-SH) and chitosan polymers deposited on the surface of GNPs play on their optical properties. We also study GNP configurations which gradually shift from isolated particles toward connecting particles and infer their LSPR and SERS activity.

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AB INITIO STUDY OF OPTICAL ABSORPTION AND ELECTRON ENERGY LOSS SPECTRA OF SWCNTs

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Optical properties of SWCNTs are powerful means for determining their structures. We present results for the optical absorption and electron energy loss spectra of Single-Walled Carbon nanotubes (SWCNTs) obtained by ab initio calculations in the framework of density functional theory (DFT) [1]. Optical transitions in SWCNTs, together with their Raman spectra, provide a tool for assigning the structural parameters of a certain nanotube. We calculate first, second, and third optical transitions in several SWCNTs. We also address electron energy loss spectra for these systems. The calculated optical spectra are in excellent agreement with available experimental data. Unlike the larger diameter carbon nanotubes whose absorption spectra are insensitive to the tube chiralities, the absorption spectra of 4 Å Single-Walled Carbon Nanotubes depend very much on their chiralities. The dielectric function was found highly anisotropic being much larger when the electric field is aligned along the tube axis than when it is aligned perpendicular to the tube axis.

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