

# Terahertz Resonant Dipole Nanoantennas

Salvatore Tuccio<sup>1</sup>, Alessandro Alabastri<sup>1</sup>, Luca Razzari<sup>1</sup>, Andrea Toma<sup>1</sup>, Carlo Liberale<sup>1</sup>, Remo Proietti Zaccaria<sup>1</sup>, Francesco De Angelis<sup>1</sup>, Gobind Das<sup>1</sup>, Enzo di Fabrizio<sup>1</sup>

<sup>1</sup>Istituto Italiano di Tecnologia, Genova, Italy

## Abstract

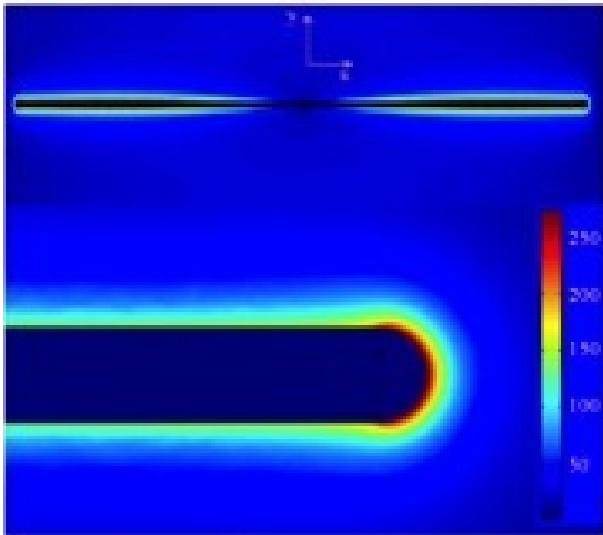
Introduction: Nanoantennas have been successfully employed for single-molecule spectroscopy [1], chemical mapping [2], optical microscopy [3], solar energy conversion [4] and nonlinear optics [5]. Their distinguishing feature consists in strongly enhancing the light-matter interaction at the nanoscale and in converting the free propagating radiation into a highly localized optical field [6]. So far, most of nanoantenna applications have been principally confined to the visible and infrared regions of the electromagnetic spectrum. Here we show the possibility to expand usual nanoantenna functionalities in the THz domain, making use of a gold nanostructure, in the typical form of a dipole nanoantenna, able to resonate in the THz frequencies range. In this work we considered an array of aligned planar gold nanoantennas over a silicon substrate. Important near field and far field properties were obtained with FEM simulations. The high values of the near field intensity enhancement, strongly localized at the device ends, as well as of the extinction efficiency indicate direct applications in material science and potential uses for THz spectroscopy and nonlinear optics. Use of COMSOL: Relevant electromagnetic properties of the THz resonant dipole nanoantennas were calculated in the frequency domain with numerical simulations performed using the scattered field formulation available in the COMSOL's RF Module. The nanoantenna is modeled as a rod with rectangular section (width  $W=200\text{nm}$ , height  $D=60\text{nm}$ ) with hemicylindrical end caps of radius  $R=100\text{nm}$  and total length of  $L=40\ \mu\text{m}$  [7]. All sharp edges are blended (radius of curvature  $r=20\ \text{nm}$ ). The dielectric constant of gold is taken from [8]. In the simulations, the nanoantennas are embedded in an effective medium whose permittivity is calculated as the mean value of the dielectric constant of the substrate and that one of air. Periodic boundary conditions are considered to represent the behavior of a periodic array, with a distance of  $20\ \mu\text{m}$  in the orthogonal directions. The system is illuminated at normal incidence with a plane wave polarized along the long axis of the nanoantennas. Far field properties of the gold nanoantennas are quantified in terms of calculated dimensionless absorption and scattering efficiencies  $Q_{\text{abs}}=P_{\text{abs}}/\sigma_{\text{geo}}$  and  $Q_{\text{sca}}=P_{\text{sca}}/\sigma_{\text{geo}}$  where  $\sigma_{\text{geo}}$  is the geometrical cross section of the nanoantenna) and resonance frequency position,  $P_{\text{abs}}$  is obtained by integrating the resistive losses in the total volume of the nanoantenna and  $P_{\text{sca}}$  is calculated by integrating the time averaged outgoing power flow of the relative fields on a closed surface that contains the scatterer. Results: Figure 1 shows the absolute value of the electric field around the nanoantenna on a cut plane normal to the direction of the illuminating wave, exactly positioned at the antenna half height. The field is highly localized at the nanoantenna ends. The field enhancement factor  $F$  as a function of frequency is reported in Figure 2. A wide resonant behavior can be observed, with a maximum enhancement value of about 280 at around 1.3 THz. The full width at half maximum of the field distribution 1 nm away from the nanoantenna

end is 180 nm (inset in Figure 1). This means that the structure successfully concentrates the radiation on a later size smaller than  $\lambda/1000$ . Figure 3 represents the spectra of the extinction, absorption and scattering efficiencies. The extinction efficiency shows a maximum value of around 110 at the resonance frequency. Conclusion: The high field enhancement could be successfully employed for the detection of few molecules with THz spectroscopy, since the effective absorption cross section of a molecule close to the nanoantenna scales with  $|F^2|$  and would then be enhanced by several orders of magnitude at the antenna ends. In addition, nonlinear interactions at THz frequencies, usually difficult to be observed due to the low intensity of the available THz sources, can be strongly enhanced by resonant nanoantennas.

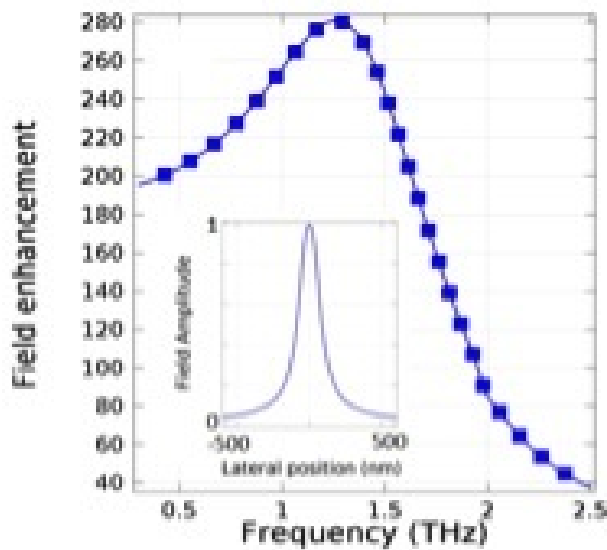
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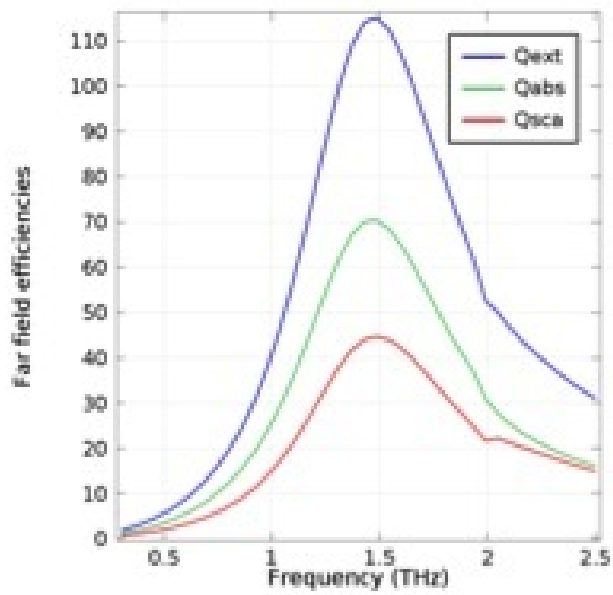
## Figures used in the abstract



**Figure 1:** Contour plot of the absolute value of the electric field around the nanoantenna under resonant condition. Upper part: overall device, lower part: magnification at the end.



**Figure 2:** Field enhancement factor  $F$  at the nanoantenna end as a function of frequency. Inset: normalized electric field profile close to the nanoantenna end. The values of the field are calculated along a line perpendicular to the long axis of the antenna at a distance of 1 nm.



**Figure 3:** Spectra of the efficiency of scattering  $Q_{sca}$  (red), absorption  $Q_{abs}$  (green) and extinction  $Q_{ext}$  (blue). Extinction efficiency is calculated as:  $Q_{ext} = Q_{sca} + Q_{abs}$