ADVANCED OPTICAL MATERIALS

Supporting Information

for *Adv. Optical Mater.,* DOI: 10.1002/adom.202000769

All-Optical Polarization-Controlled Nanosensor Switch Based on Guided-Wave Surface Plasmon Resonance via Molecular Overtone Excitations in the Near-Infrared

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All-Optical Polarization-Controlled Nanosensor-Switch Based GWSPR via Molecular Overtone Excitations in Near-Infrared

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All-Optical Polarization-Controlled Nanosensor-Switch Based GWSPR via Molecular Overtone Excitations in Near-Infrared

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S1. GWSPR Performance

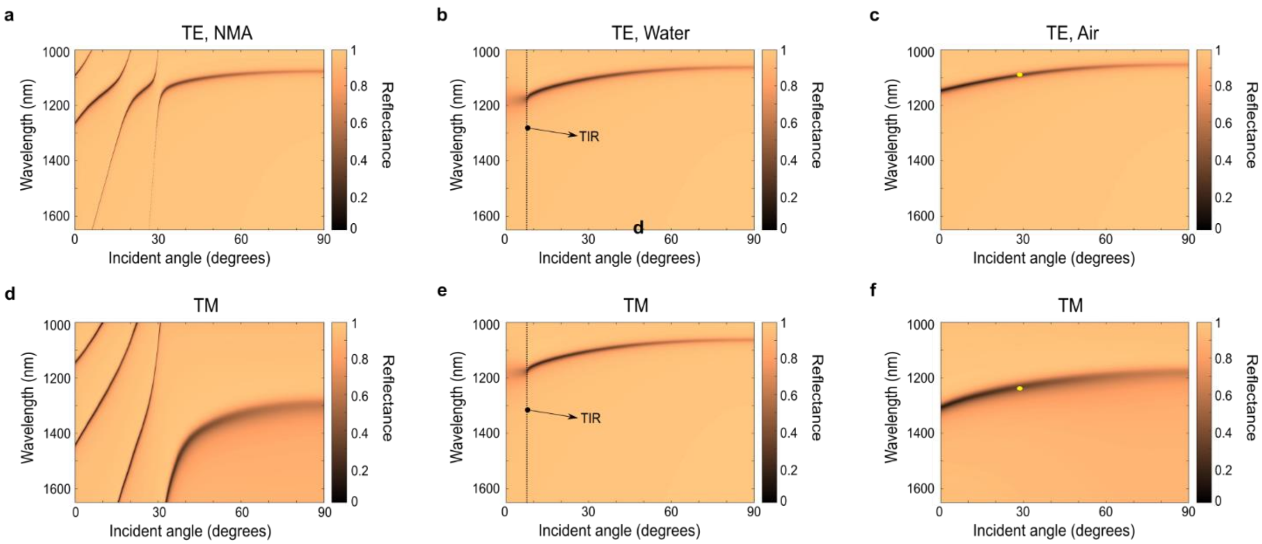

Figure S1 | Dispersion colormap of GWSPR. a-f) Calculated results of Abeles-matrix based algorithm implemented in Matlab of multilayer structure consisting of SF-11 glass substrate covered by 18 nm silver (Ag) under 219 nm silicon (Si) film and 32 nm of silica (SiO_2). The thickness of N-SF11 glass in the simulation is semi-infinite; dispersion colormap of a multilayer structure with superstrate medium of N-Methylaniline (NMA) molecule excited by **a**) TE and **d**) TM polarized light; calculated results in **b**) TE and **e**) TM of the multilayer structure when water is the superstrate medium with a refractive index of 1.33; the dispersion colormap in **c**) TE and **f**) TM with air as a superstrate medium, the obtained calibration measurements carried out with the fabricated device were marked with yellow dots.

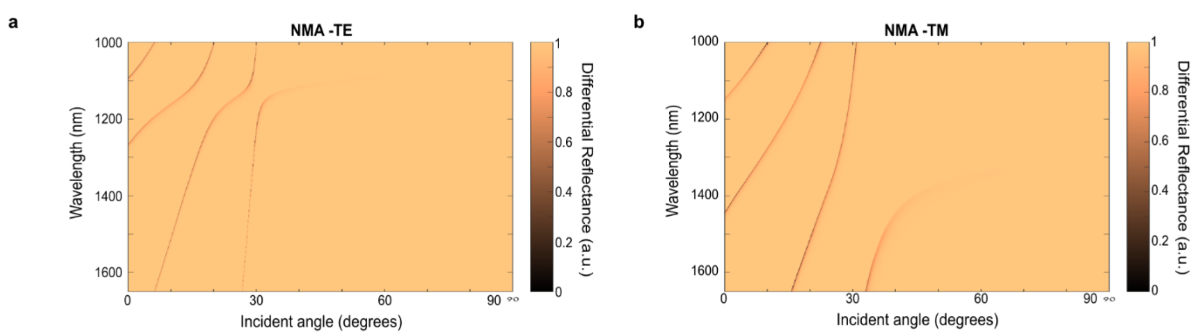

Figure S2 | Differential reflectance. a-b) Calculated results of reflectance normalized to the background of the GWSPR structure, using equation (4) in the Experimental Section. With 1600 nm film of NMA molecule and superstrate medium of air excited by **a**) TE and **b**) TM polarized light.

Figure S1 show the dependence of both the wavelength and the incidence angle in reflectivity of the GWSPR configuration with different analyte materials for both TE and TM polarized light. To better explore the excitation behavior of ESPs coupled to the waveguide modes, in our study the reflectivity was calculated in MATLAB® environment using the Abeles matrix method. Due to using GWSPR configuration guided-modes evolve in addition to the SPR mode, multiple resonances can be observed in the reflectivity. The multiple resonances are clearly described by the black curves created in Figures S1a,c. Note that the additional resonances attributed to guided-modes rather than to ESPs mode. Figure S1c,f additionally represent the measurements (yellow dots) were carried out in the fabricated GWSPR model, the resonances obtained appears to be compatible with the calculated dispersion maps.

S2. Calibration of The Optical System

Designing of a numerical tool for the coupled three-resonator system requires consideration at all the optical phenomena occurring, in order to allow the ability for detection and sensing. Accordingly, it is necessary to operate in several steps. First, we deal with the NGSPR configuration to excite an SPP wave, it is the main aim, provide an indication of the numerical tool compared to the sensor performance with consideration of the fabricating process by electron-beam physical vapor deposition (EBPVD).

To examine the behavior of the sensor, the colormap in Figure S3a show the reflectance as a function of both the wavelength and the incidence angle. The reflectance of NGSPR configuration was calculated numerically in Matlab environment based on the Abeles matrix method. We developed the NGWSPR model which formerly investigated for detection of molecular overtone transitions, consist of an SF-11 prism coated by a silver layer with a 10 nm thin film of silicon for detection water. The optimal silver layer thickness achieves resonance in the NIR is 50 nm, while $R_{min} \approx 0$ and the incident light is TM polarized.

In this proceeding, to satisfy the conditions for excitation of plasmons we used a collimated beam incident on the coupling prism from a polychromatic light source trough TM polarizer. The prism match between both ***k*** vector of the plasma and the incident light, located on the rotation stage which allows us to measure with various angles. Noted, since the physical limitation of the prism, extremely small, should considering small angles. The fabricated sample was placed on the prism when matching oil located between them, while the water dripped on the top surface. Using a diverging lens, the reflected beam from NGWSPR structure collected inside fiber and directly to the optical spectrum analyzer. The observed SPR signal measurements of the reflectance shown in Figure S3b together with calculations performed by the numerical tool. One can clearly see the matching between these results, in addition, as expected a redshift of the resonances was seen while decreasing the incident angle.

Then, we expanded the numerical tool for the GWSPR configuration which allows the polarization-controlled incident light for exciting ESP coupled to guided wave, allowing us broad investigation and collecting more information from the analytical material. We tuned the thickness of the layers, expressly, silver layer to 18 nm, increase the silicon layer to 219 nm and 32nm of SiO_2 was added on the top layer, to receive the multiple resonance phenomenon around the first and second overtone regions of the probing NMA molecule. The optimization, fabrication, and the experimental setup of GWSPR model were based on the same principles in NGSPR case. To simulate the hybrid overtone-plasmon system completely firstly we used COMSOL Multiphysics 5.4 with optics wave model for the GWSPR model in the wavelength domain. It is necessary to calibrate all models together for comparison, the results of the numerical tool, the COMSOL simulation, and of course measurement achieved with the fabricated model for air. Figures S3c,d show a classic match between the numerical tool and the simulation considering the measurement results were obtained.

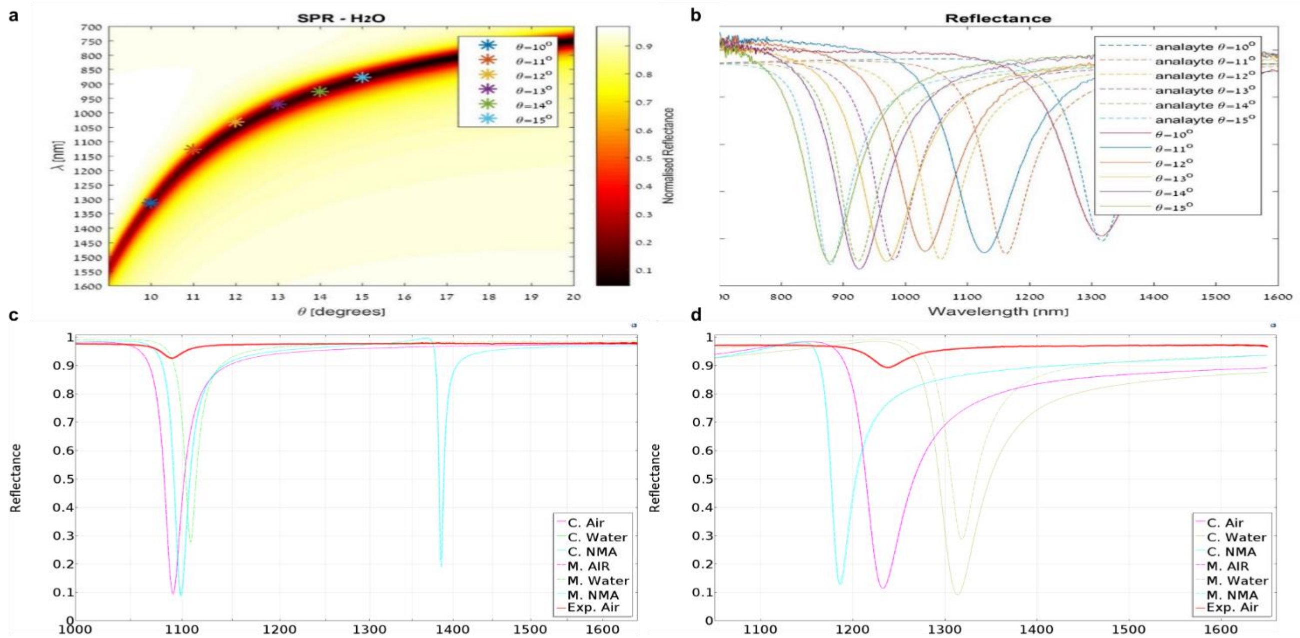

Figure S3 | Calibration of the optical system. a) Dispersion colormap of NGSPR model as a function of both wavelength and incidence angle, the stars represent the measurements obtained for different angles with the fabricated sample. **b)** Numerical results (dashed lines) and experimental measurements (solid lines) for various angles of the incident light, each curve describe the wavelength dependence of reflectance at a fixed angle for 10, 11, 12, 13, 14, and 15 degrees from right to left, respectively. **c,d)** Wavelength-dependent the reflectance of GWSPR configuration for air, water, and N–Methylaniline (NMA) molecule, at 28.7 degrees for **c**) TE and **d**) TM polarized light. Including the SPR measurements of the fabricated model obtained for air (red).

The optical properties defined completely by the dielectric constant, which can be realized by using the Drude-Lorentz model. Different researches describe a modification on the dielectric constant depending on the thickness of the silver film that deposited on silicon substrates by a conventional EB-PVD. Here, due to using the EB-PVD process can assume this effect on the silver film in our GWSPR model which deposited on an SF11 glass substrate. Thus, can easily obtain a match between the numerical tool and the measurements achieved. In the case of silicon, we used an empirical dielectric constant model which also produces changes. Figure S4 show the distributions of n and k of the refractive index, for (left y-axis) silver and (right y-axis) silicon films. One can see clearly the increase in both n and k compared to those of the Drude-Lorentz model. It can be achieved by tuning the multiplication factor of both parts, the real and the imaginary. Expressly, in this case, the optimal factors are ${n_{Ag}}_{\mathrm{Drude-Lorentz}} = n + i\kappa \rightarrow {n_{Ag}}_{Optimal} = 2 \cdot n + 1.3 \cdot i\kappa$ for silver and ${n_{Si}}_{\mathrm{D}} = n + i\kappa \rightarrow {n_{Si}}_{Optimal} = 1.1 \cdot (n + i\kappa)$ for silicon. However, based on the modifications in optic properties of the materials, and synthesis of the nanorod, the complete hybrid three-resonator system can be handled with the numerical tools that were confirmed in this work. Namely, adding nanorod on the top surface of the GWSPR model.

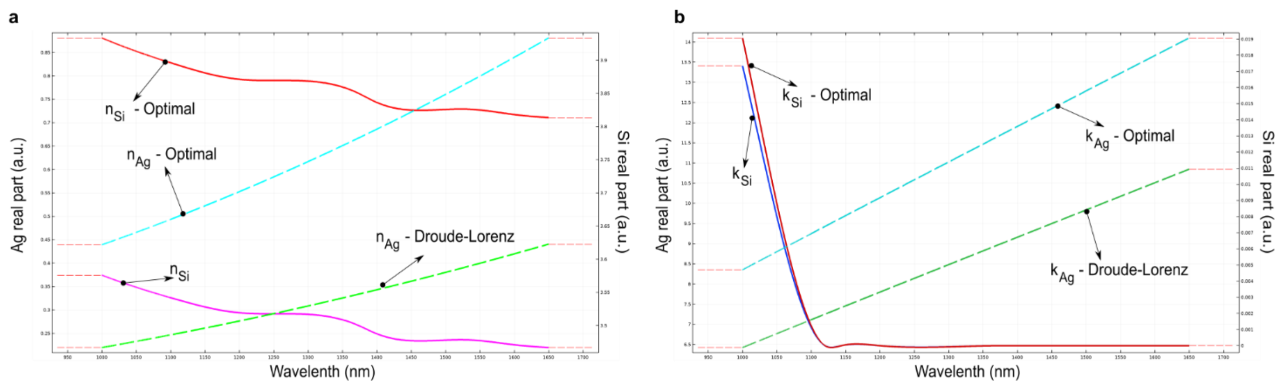

Figure S4 | Optical characteristics a,b) The distributions of **a**) n and **b**) k of the refractive index, $\tilde{n} = n + ik$, for silver and silicon films. One can see the changes between the optimal n and k, compared to those of the Drude-Lorentz model, in particular, multiplying a constant with the real and imaginary parts of the refractive index for both silver and silicon. The left *y*-axis represents the values for silver and right *y*-axis for silicon.

S3. The hybrid plasmonic-dielectric arrangement

According to Figure 5a of the main text, the system is illuminated by TM (Figure 5a top) or TE (Figure 5a bottom) polarized incident beam when incoming light hits the prism left facet as indicated by the ***k*** vector direction. Whereas the intensity of the reflected beam is collected from the right facet. We note, that the coordinate system is located in the middle, where the nanorod is positioned at the silica-NMA molecule interface with the nanorods oriented with *x*-axis. The electric far-field radiation was calculated at different angles between the nanorods for 0° to 15°, where α is the angle created by the x-axis and the top nanorod with clockwise rotation as shown in Figure S5a.

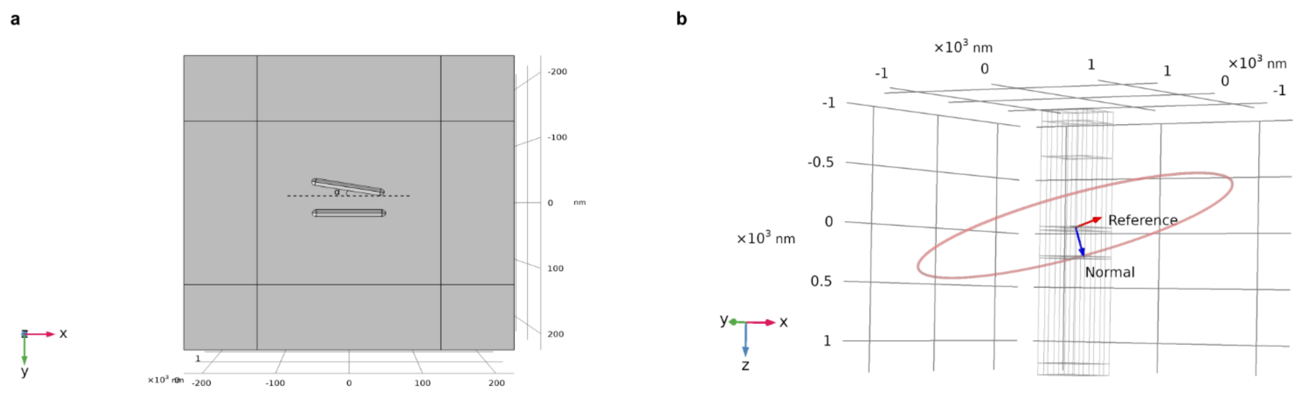

Figure S5 | The nanorods orientation. a) The nanorods order on top of the GWSPR configuration which is embedded in weakly NMA absorbing medium with different angles between the nanorods. **b)** 2D patterns classification of the far-field radiation when the normal in the xz-plane and the reference direction in the x-axis for both 'on' (TM polarization) and 'off ' (TE polarization) switching states at 1500 nm when a unit cell of the system represented.