Supplementary Information

Higher order Fano graphene metamaterials for nanoscale optical sensing

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Simulation method for transmission spectra

Considering the 3D FEM calculated amount and the mesh quality, the smallest mesh size of graphene is 0.5 nm and the mesh size gradually increases outside the graphene layer, which can reach proper convergence. In addition, the graphene layer is ultra-thin, which is treated as the inner boundary conditions (transition boundary condition) with the thickness 1 nm in our simulation.

In the the simulation, the periodicity of the metamaterials (P = 300 nm) is much less than the resonance wavelength (around 7~10 μm), thus there isn't the high order diffraction. Hence the transmission (T) data is extracted from the S21 parameter:[1]

$$T = |S_{21}|^2$$

The definition of the S-parameters in terms of the power flow is:

$$S_{21} = \sqrt{\frac{\text{Power delivered to port 2}}{\text{Power incident on port 1}}}$$

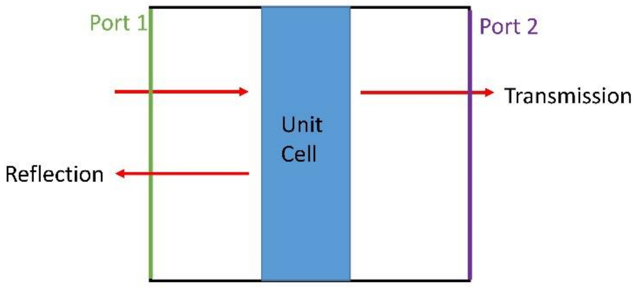

Fig. S1 Schematic illustration of the transmission data is extracted by the FEM simulation.

The effect of the closest separation in SRR/disk

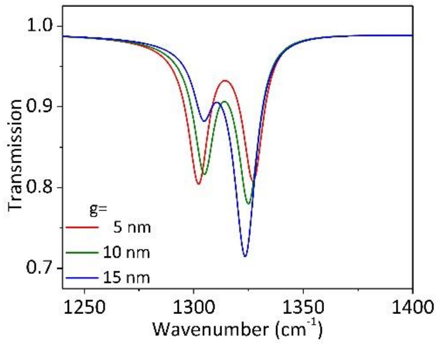

Fig. S2 Transmission spectra of the HC Fano resonance structure with the closest gap varied from 5 to 15 nm, and the Fermi energy is 0.5 eV.

The Fano resonance is still obvious when the nanogap is below 15 nm in our structure as demonstrated in Fig. S2. With the nanogap increasing from 5 to 15 nm, the coupling efficiency of the Fano resonance would decrease, but the pure higher order graphene Fano resonance is still created to avoid the crosstalk in refractive-index sensing. Thus, the closest gap can be selected more than 5 nm in the experiment. In addition, with the rapid development of nanofabrication technologies such as focused ion beam (FIB) and electron beam lithography (EBL), the accuracy of nanogap would become higher. The smallest nanogap has been realized around 1.5~10 nm by FIB[2] and 4 nm by EBL[3]. Hence we think it is possible to fabricate the metamaterials with the rapid development of nanofabrication technologies.

Notes and references

1. J. S. Gomez-Diaz and J. Perruisseau-Carrier, *Opt Express*, 2013, 21, 15490-15504.
2. M. D. Fischbein and M. Drndić, *Nano letters*, 2007, 7, 1329-1337.
3. Y. Sonnefraud, N. Verellen, H. Sobhani, G. A. Vandenbosch, V. V. Moshchalkov, P. Van Dorpe, P. Nordlander and S. A. Maier, *ACS nano*, 2010, 4, 1664-1670.