Electronic Supplementary Material (ESI) for Lab on a Chip.
This journal is © The Royal Society of Chemistry 2014

Supplementary information

1. Simulation method

For a particle trapped by a highly localized field, as the case in our work, it is more appropriate to calculate the induced optical force by using Maxwell stress tensor (T_M). In our simulations we first model the designed structures, and set the object (particle) at a position we are interested in. Then we launch waves and simulate the resulting distribution of optical field in steady state. With the field distribution, we can calculate the optical forces. Maxwell stress tensor is a vectorial surface density of optical force. In Cartesian coordinate, each component of the time averaged force density can be expressed as:

$$< T_{Mx} > = \frac{1}{2(particle\ radius)} *$$

$$\begin{pmatrix} x * real[conj(E_x) * (D_x)] + x * real[conj(H_x) * (B_x)] \\ -\frac{1}{2} * x * [conj(E_x) * (D_x) + conj(E_y) * (D_y) + conj(E_z) * (D_z)] \\ -\frac{1}{2} * x * [conj(H_x) * (B_x) + conj(H_y) * (B_y) + conj(H_z) * (B_z)] \\ + y * real[conj(E_y) * (D_x)] + y * real[conj(H_y) * (B_x)] \\ + z * real[conj(E_z) * (D_x)] + z * real[conj(H_z) * (B_x)] \end{pmatrix}$$

$$< T_{My} > = \frac{1}{2(particle\ radius)} *$$

$$\begin{pmatrix} x * real[conj(E_x) * (D_y)] + x * real[conj(H_x) * (B_y)] \\ + y * real[conj(E_y) * (D_y)] + y * real[conj(H_y) * (B_y)] \\ -\frac{1}{2} * y * [conj(E_x) * (D_x) + conj(E_y) * (D_y) + conj(E_z) * (D_z)] \\ -\frac{1}{2} * y * [conj(H_x) * (B_x) + conj(H_y) * (B_y) + conj(H_z) * (B_z)] \\ + z * real[conj(E_z) * (D_y)] + z * real[conj(H_z) * (B_y)] \end{pmatrix}$$

$$< T_{Mz} > = \frac{1}{2(particle\ radius)} *$$

$$\left\{ \begin{array}{c} x * real[conj(E_x) * (D_z)] + x * real[conj(H_x) * (B_z)] \\ + y * real[conj(E_y) * (D_z)] + y * real[conj(H_y) * (B_z)] \\ + z * real[conj(E_z) * (D_z)] + z * real[conj(H_z) * (B_z)] \\ - \frac{1}{2} * z * [conj(E_x) * (D_x) + conj(E_y) * (D_y) + conj(E_z) * (D_z)] \\ - \frac{1}{2} * z * [conj(H_x) * (B_x) + conj(H_y) * (B_y) + conj(H_z) * (B_z)] \end{array} \right\}$$

,where **E** is the electric field, **D** is the electric displacement field, **H** is the magnetizing field, and **B** is the magnetic field. The subscript indicates each component of projection in Cartesian coordinate. In Comsol Multiphysics we can select the boundary of the particle and directly insert the above expressions into a space at the interface for performing boundary integration. The integration results representing each force component can be obtained promptly. By changing location of the particle and repeating the simulation process, we can obtain the force on the particle as a function of the location. The potential energy in integration form, $U(r) = -\int_{\infty}^{r} F(r') \cdot dr'$, can be used to calculate the potential energy experienced by the particle at location ***r***, where ***r*** and ***r'*** are position vectors of the particle. This is a path integration, which represents the loss of potential energy when the particle moves from somewhere far away to the center of the trapping site. Finally we can determine whether the particle can be stably trapped by depth of the potential well. It had been proposed by Ashkin *et al.* in 1986 that a sufficient trapping condition requires the Boltzmann factor exp($-U/k_BT$) much smaller than one, where U is the potential of the trapping force [18]. This is equivalent to requiring that the time to pull a particle into the trap be much less than the time for the particle to diffuse out of the trap by Brownian motion, which is random motion of particles suspended in fluid (liquid or gas) resulting from their collision with the quick atoms or molecules in the medium. They claim $U/k_BT \geqq 10$ as the criterion which guarantees stable trapping of particle. This had been widely used in many works to determine whether the design of optical trap can hold the particle unaffected by Brownian perturbation [3, 19].

2. Comparison of different gap sizes

It had been shown that the LSPR mode in bowtie of smaller gap can induce stronger trapping force due to the better electric coupling across the gap. For better understanding, here we show the field distributions for 30 nm and 5 nm gap sizes at the plane of x = 0 (Figs. S1(a) and (b)). The profile of particle can be seen by the transition of field strength across the boundary. It is obvious that the field strength within the 5 nm gap is much stronger and the particle is of significant overlap with the resonant field. Therefore the bowtie of 5 nm gap can induce stronger optical trapping force on the particle than those of wider gap sizes.

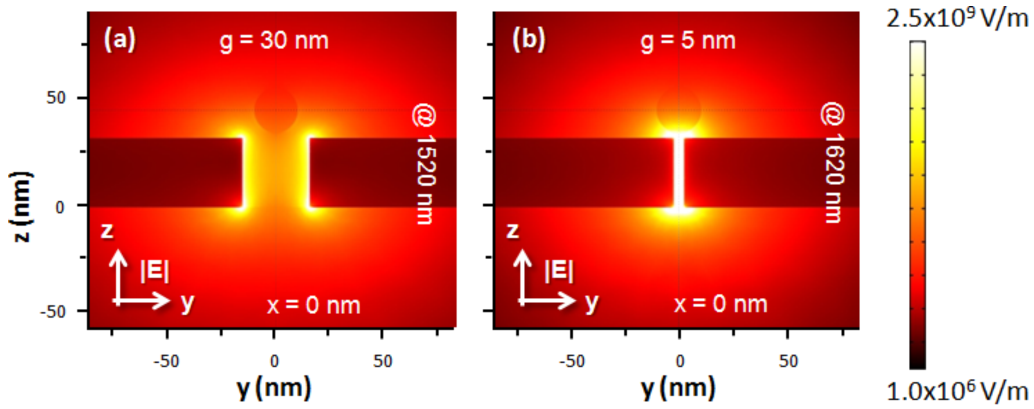

Fig. S1: Field distributions of the LSPR modes for the bowties with gaps of (a) 30 nm and (b) 5 nm, respectively, at the plane of x = 0.