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# تشدید پلاسمون سطحی در نانو ساختار فلزی جهت تشخیص ملکول DNA

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چکیده – اثر اندازه و فاصله در نانو ذرات پروانه‌ای شکل بر تشدید پلاسمون سطحی در نواحی ماوراء بنفش و نور مرئی به روش تقریب گسسته دو قطبی، مورد بررسی قرار گرفته است. یکی از جنبه‌های بسیار مهم این فعالیت نظری در نحوه‌ی تغییر مدهای تشدید پلاسمون سطحی در نانو ذرات بعد از نزدیک شدن ملکول DNA به ساختار می‌باشد. محاسبات نشان می‌دهد که تشدید پلاسمونی آشکار شده در نانو ذرات طلا، به صورت فزآینده‌ای به طرف باند قرمز جابه‌جا می‌شود. حساسیت ساختار مبتنی بر طلا به ملکول DNA به ترتیب برای حالت عمودی و افقی حدود ۰،۰۵ و ۰،۰۱۸ است، اما ساختار آلومنیومی حساسیت بسیار کمتری در مقایسه با طلا دارد. ساختار پیشنهادی قابلیت تشخیص عبور و همچنین نحوه عبور افقی و عمودی ملکول DNA را دارد. نتایج بدست آمده ساختار پروانه‌ای طلا را جهت توسعه بیو سنسورهای تشخیص دهنده و توالی یابی DNA بسیار مناسب نشان می‌دهد.

کلید واژه- نانو ساختار، بیو سنسور، تشدید پلاسمون سطحی، تقریب گسسته دوقطبی

# Surface Plasmon Resonance of Metal Nanostructures for Sensing DNA

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Abstract- Metallic bowtie nanostructures (BNSs) and their surface plasmon resonance (SPR) properties in the UV/Vis region, for Al and Au materials, have been investigated by employing discrete dipole approximation method. A crucial aspect for these applications is how SPR in BNS is affected after approach with DNA molecule. Our results reveal that SPR in Au nanostructure is redshifted by the DNA present. Au-based BNS have sensitivities about 0.055 and 0.018 to the vertical and horizontal DNA molecules, respectively. But sensitivity of Al-based BNS is very smaller than the Au. Moreover, DNA passage and its vertical and horizontal nature through the gap can be determined by the proposed method. Results provide useful indications for future characterization and monitoring of DNA molecules via SPR properties of nanostructures, as well as for the development of biosensing, trapping and sequencing devices.

Keywords: Nanostructure, Biosensor, Surface Plasmon Resonance, Discrete Dipole Approximation

# Surface Plasmon Resonance of Metal Nanostructures for Sensing DNA

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## 1 Introduction

Metal nanoparticles (NPs) play a prominent role in nanotechnology due to their favorable combination of physical–chemical properties [1, 2]. Eextensive investigations of surface plasmon resonance (SPR) properties and their applications have focused on metallic nanostructures, such as Au, Ag, and Cu [3]. There have been few studies on SPR in the ultraviolet (UV)-light region [4]. Non-noble metals, such as Al, are one of the best candidates for deep-UV and longer wavelength applications because the SPR is more pronounced and can be tuned over a broad wavelength range [4, 5]. The arrangement of metal nanostructures lead to plasmonic properties which can be utilized in biomolecule sensing. The coupled plasmon modes between nanostructures are very sensitive to the gap distances and the particle nature [4, 6, 10]. For DNA detection, blueprint of life, bowtie structure is the best candidate [4]. Among various designs, plasmonic particles consisting of adjacent metallic nanoparticles with nanoscale gaps have shown extremely strong field confinement and enhancement in the gap regions due to the in-plane near-field coupling across the gaps [4].

Here we use discrete dipole approximation (DDA) method [7] to study SPR in bowtie nanostructures (BNSs) in the proximity of DNA or embedded in BNS. Our calculations show that SPR is sensibly influenced by the presence of DNA.

## 2 Materials and Method

Proposed structures are shown in Figures 1a, b and c, BNS, BNS with vertical DNA and BNS with horizontal DNA molecule presented, respectively. To study SPR properties of the proposed structures, we use DDA method. In recent years, DDA has been developed for calculating SPR properties for isolated nanoparticles of arbitrary shapes, complex surrounding environments, and sizes on the order or less than the incident light wavelength [7]. The DDA method calculates scattering and absorption of electromagnetic radiation by dividing the object of interest into a cubic lattice of *N* dipoles [7].

$$C_{ext} = \frac{4\Pi k}{|E0|^2}\sum_{i=1}^{N} Im(E^*_{loc,j} \cdot p_j) \quad (1)$$

$$C_{abs} = \frac{4\Pi k}{|E0|^2}\sum_{i=1}^{N}\{Im[p_j.(\alpha_i^{-1})^* p_i^*] - \frac{2}{3}k^3 |p_i|^2\} \quad (2)$$

The terms $E_0$ and $k$ are the amplitude and wave vector of the incident light, respectively. The $P$ is dipole moment vector, $\alpha_i$ is polarizeability and extinction and absorption efficiencies are evaluated as $Q_{ext} = C_{ext}/\pi_{aeff}^2$ and $Q_{abs} = C_{abs}/\pi_{aeff}^2$, respectively, where the effective radius $a_{eff}$ is defined through the concept of an effective volume equal to $4\pi_{aeff}^3/3$. For the calculations, we used DDSCAT code [7]. For modelling Au, Al and DNA in the DDA method, we use dielectric functions presented in [8] and [9], respectively.

## 3 Results and Discussion

A plane-wave source was illuminated to the structure, and the direction of the propagation of the source is the direction of the structure thickness (x axis in Fig. 1). The direction of the electric field was parallel to the Z axis. Figure 2 shows extinction efficiency spectrums for Al- and Au-based BNSs. Al-based BNS with parameters of $a$ = 18, $b$ = 18 and $c$ = 10 nm, in Fig. 1 a, shows an extremely strong and narrow peak around 170 nm Figure 2a.By decreasing of gap length from 7 to 2 nm a new peak is appeared in 290 nm, results show that second peak is redshifted by decreasing gap length. Then, the electric field enhancement factor (EFEF), which is defined as ($|E|^2$ / $|E|_0$), was calculated for Al-BNS structure, Figure 3. A comparison with the Au structures, Figure 2b and c, reveals that the Al-based SPR wavelength is far shorter than that of Au. The SPR wavelength for Au is 530 nm, whereas the SPR wavelength of Al is about 170 nm and located in deep-UV region. In addition, decrease in gap distance causes redshift in the resonance peak of Au and the peak of Al around 250 nm. The fixed wavelength of the Al-based BNSs corresponding to the gap distance

changes, is related to the triangles, individually. But the peak with larger wavelength is related to the coupled mode between them which is more affected by the gap distance. In the second approach to investigate effects of biomolecules on the SPR of BNSs, we considered the ideal case of a DNA, modelled as a nano cylinder with diameter $d$ = 5 nm and length of 10 nm located in the gap, Figure 1b. In addition, DNA is presented to the gap in vertical and horizontal placement, as it can be seen in Figures 1b and c. To study viability of the proposed structure for DNA sensing, we define sensitivity factor as[6]

$$SF = \sum_j^M \frac{|\lambda_j - \lambda_{j,No\ DNA}|}{\lambda_{j,No\ DNA}} \quad (3)$$

Where $M$ is the total number of SPR modes, $\lambda_j$ and $\lambda_{j,No\ DNA}$ are the peak wavelengths for the mode number $j$ while DNA molecule present and no DNA is presented, respectively. For Au structure and for the vertical and horizontal DNA molecules, sensitivity factors are 0.055 and 0.018, respectively. Generally, absolute value of the sensitivity is relative to the length of the DNA molecule. In this part, we considered a DNA molecule of 10 nm length. Al-BNS cannot distinguish between horizontal and vertical DNA molecules, figure 4a. But peaks related to the Au-BNS with vertical and horizontal DNA molecules takes about 20 nm relative shift, Figure 4b. However, Al sensitivity is very small compared to Au. This is in good agreement with the previous studies on the Al-BNSs for sensitivity of biomolecules which shows small sensitivity for Al. Despite technical challenges, such as fabrication process, relatively small bowtie structures of Au show a great potential to be used in sensing and sequencing amplified DNA molecules and their nucleotides. Also, we should note that recent studies on the bowtie structures suggest that they can be used simultaneously as a sensing and speed-control device while DNA molecule passes vertically through the gap.

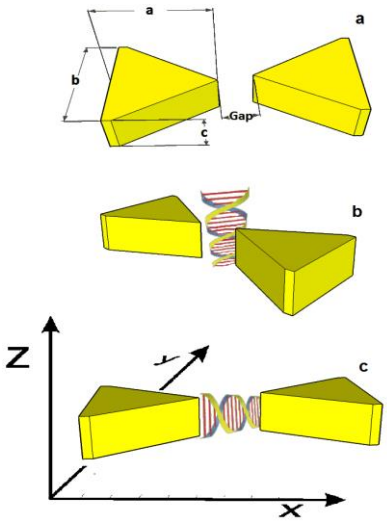


Figure 1. (a) BNS geometry and DNA molecule presented (b) vertical and (c) horizontal to the gap

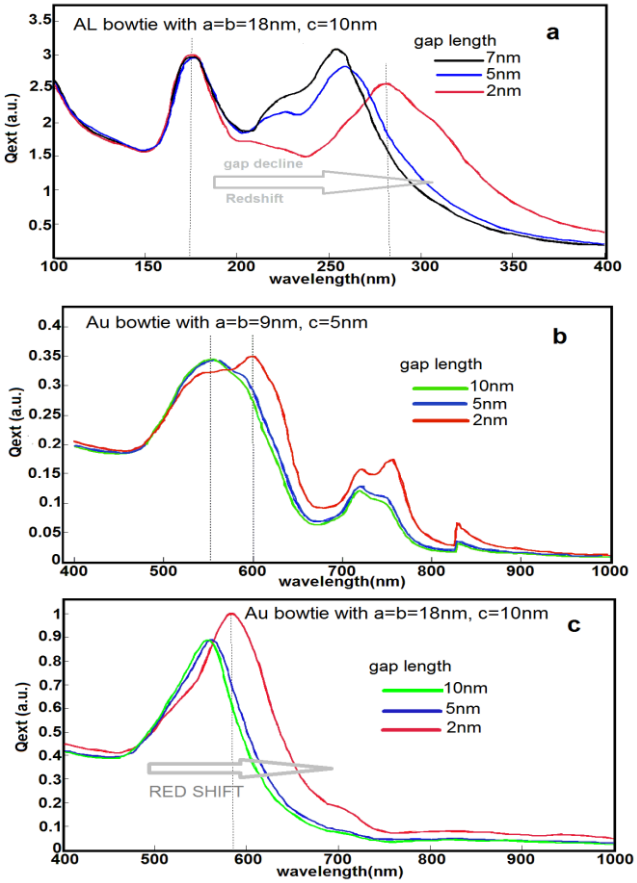


Figure 2. $Q_{ext}$ for: (a) Al-BNS with different gap distances, , (b) Au-BNS with different gap distances and (c) Au-BNS with increased sizes and different gap distances

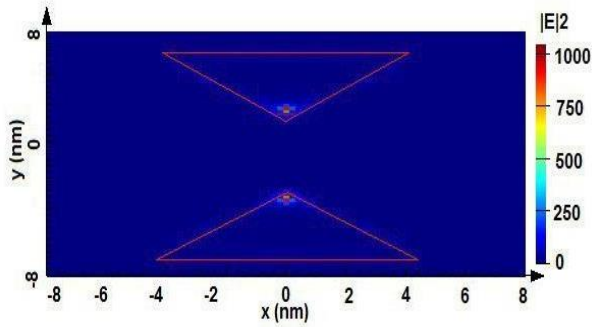


Figure 3. EFEF factor calculated. the

Structure were Al-based with a=b=18nm, c=10nm and 7nm gap length

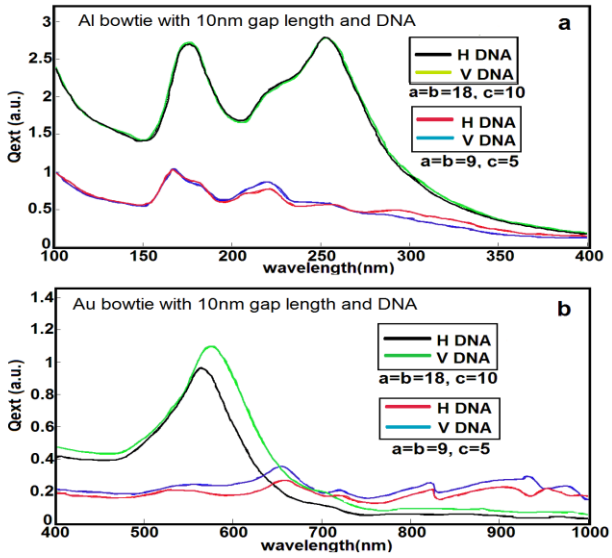


Figure 4. $Q_{ext}$ for (a) Al-based and (b) Au-based BNSs with DNA in vertical (V) and horizontal (H) placement

## 4 Conclusion

In summary, we study SPR properties of BNSs in the proximity of DNA, embedded horizontally or vertically in the gap, utilizing the DDA method. The effects of size, shape and gap of the BNSs were investigated. Redshifts in the coupled modes of both Al- and Au-based structures by decreasing gap distance are seen. Results show that the SPR of Au-based bowtie by proximity of DNA redshifts until the length of the structure is comparable with DNA. The Au-based BNS shows sensitivities about 0.055 and 0.018 to the vertical and horizontal DNA molecules, respectively. The Al sensitivity is very small compared to Au. Proposed method can detect DNA passage event and behavior through the gap. Our results provide useful indications for characterization and monitoring of DNA molecules via SPR properties of nanostructures.

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