




# Charge transfer plasmon resonances of conductively linked asymmetric gold nanoparticle dimers

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## Abstract

Understanding a direct transfer of charges in bridged conductive nanodimers is a central research problem relevant for numerous applications including nanomotors, sensing and other optoelectronic devices. Here we investigate theoretically the tunability of charge transfer plasmon resonances (CTPRs) of bridged symmetric and shape-asymmetric gold nanodimers through varying the geometries of the bridging nanowire and refractive index of the surrounding medium. Unbridged symmetric dimer supports a single dipolar bonding plasmon mode, whereas two new resonance modes emerge in bridged shape-asymmetric dimers. In particular, due to the broken symmetry bridged shape-asymmetric dimer supports a sharp Fano-like resonance in the visible region. Varying the junction diameter and length of the bridging nanowire controls the resonance wavelengths and the scattering spectra of CTP modes. Increasing the diameter (length) of nanowire shifts CTP modes to considerably shorter (longer) wavelengths in the near and mid-infrared regions of the spectrum. Furthermore, the position of these resonance modes mainly depends on the refractive index of the environment, which will be useful for applications in molecular sensing. Similarly, the intensity of CTP modes can be modified by varying the aforementioned parameters. Furthermore, it was found that the CTP mode is extremely influenced by the geometries of bridged shape-asymmetric dimer. Finally, we explored the sensing applications of CTP with optimized geometries to evaluate the ability of CTP in the detection of refractive index. Hence, our designs provide extremely tunable CTP mode in the near and mid-infrared region, which are suitable for molecular sensing.

**Keywords** Charge transfer plasmon resonance · Junction conductance · Bridged nanodimers · Symmetry breaking · Sensing

## 1 Introduction

Localized surface plasmon resonance (LSPR) in nanoplasmonics is the central phenomenon that plays an important role in the operating mechanism, and performance of optical nanodevices [1]. Linked plasmonic dimers are the building blocks of optical nanodevices. Therefore, to determine their optimum performances [2–4], a comprehensive study of the optical responses of such systems is crucial for real-world applications [5]. When linked by a conductive nanojunction, this system gives rise to a novel plasmon resonance at longer wavelengths recognized as the charge transfer plasmon (CTP) [6, 7]. This new resonance mode has also been witnessed in quantum systems through the quantum tunneling due to the existence of the charge transfer [8]. A crucial distinctive characteristics related with the CTP is the oscillating electric current across the link [9]. The CTP mode keeps striking features across the mid-infrared region with great tunability by controlling the geometries

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of bridging nanowire and nanoparticles [5, 10]. A direct transfer of charges in bridged plasmonic dimers through conductive junctions acts as a fundamental component for the excitation of charge transfer plasmon (CTP) resonance [11]. Therefore, realizing these characteristics across longer wavelengths would allow for practical applications in sensing, wave-guiding, molecular electronics and building artificial molecules [5, 6, 12–15]. Understanding the CTP modes of bridged dimers through junction geometries can help researchers to attain extremely tunable plasmon resonances into the infrared region of the spectrum and it is very important for building artificial molecules, nanomotors, and other nano-optoelectronic devices [10, 15].

Recently, the optical properties of LSP resonances in bridged symmetric dimers have been comprehensively explored [5, 10] which leads to a remarkable modulation of the spectral features [6, 15, 16]. The study of the tunability of spectral features of these dimers has received growing attention due to a comprehensive range of applications in next-generation photonics technologies [17]. More precisely, radiating and nonradiating spectral features have been effectively excited and introduced by scholars such as Fano resonances [18–20], electromagnetically induced transparency (EIT) [21, 22], and charge transfer plasmons (CTPs) [12, 15]. The first two resonances can be induced based on the robust coupling of optically driven modes between proximal metallic nanoparticles (NPs) with sharp protrusions in the near-field regime [1]. In contrast, for the third resonance modes, charge transfer in particle plasmon resonances has been reported in conductively bridged NP dimers [23–26]. The CTP modes of bridged nanoparticle dimers strongly depend on the composition and morphology of the linking junction [27]. Therefore, tunable and enhanced CTP modes have been recently working for emerging ultrafast telecommunication devices, such as switches and metamodulators [11, 28]. Moreover, a direct transition of charges between the metallic nanostructures provides excellent capabilities to vigorously modulate the charge transferring through changing the intensity of the incoming light, which could be used for the progress of near-infrared and THz plasmonic nanoparticles [1].

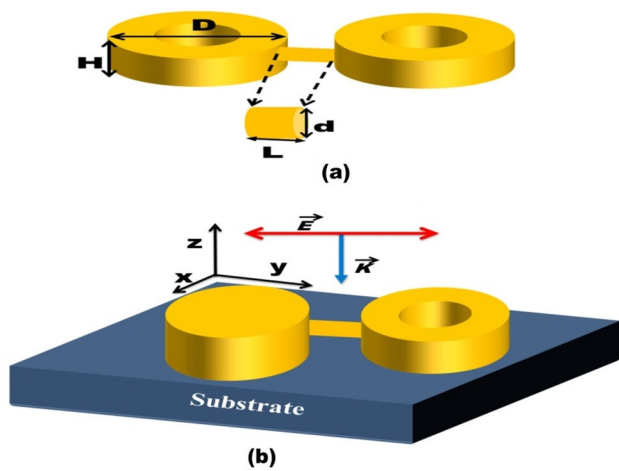
To date, numerous studies of the optical properties of bridged symmetric nanoparticle dimers have been reported on various shapes of nanoparticles such as nano core-shells [6, 29], nanodisks [24] nanoprisms [30] nanospheres [13], nanorings [5] and conductively coupled nanoparticles [10]. Nevertheless, still there is lack of complete study of the CTP modes of the linked asymmetric nanodimers. Therefore, the effect of junction geometries on the behavior of charge transfer responses of the linked asymmetric dimer has not yet been systematically explored. Furthermore, a deep understanding of the tunability of CTP modes in asymmetric dimers through the geometries of linking nanowires

is essential for real-world applications. Thus, to enhance the functionalities of bridged asymmetric dimers, a theoretical analysis of the tunability of CTP modes with varying geometries of bridging nanowires is extremely desired.

In this work, thus the effect of the junction geometry on the tunability of the CTP mode of bridged symmetric and shape-asymmetric dimers as a function of the parameters of bridging nanowires is theoretically studied. An unlinked symmetric dimer supports one dipolar bonding plasmon mode, whereas two new modes, a screened bonding dipolar mode and a low energy charge transfer plasmon mode, appear in bridged symmetric and shape-asymmetric dimers. In addition to these new resonance modes, a new Fano spectral shape is formed in bridged shape-asymmetric dimers. By controlling the junction diameter and length of the bridging nanowire we can efficiently modify the position and amplitude of CTP modes in both dimers. Increasing the diameter (length) of the nanowire shifts the CTP modes to considerably shorter (longer) wavelengths in the near and mid-infrared regions of the spectra. Moreover, the position of these resonance modes mainly depends on the refractive index of the environment, which will be useful for applications in molecular sensing. Similarly, the intensity of CTP modes can be modified by varying the aforementioned parameters. Moreover, tunability of the position and intensity of CTP mode in the bridged symmetric and shape-asymmetric dimers are systematically calculated by varying the diameter and length of the bridging nanowire. Furthermore, it was found that the CTP mode of shape-asymmetric dimer is tremendously sensitive and can be well enhanced by changing the junction diameter of the bridging nanowire. Finally, we explored the sensing applications of CTP with optimized geometries to evaluate the ability of this mode to detect the refractive index of the surrounding medium. Hence, we expect that our result is significantly important in designing tunable CTP modes in near and mid-infrared regions for practical applications in molecular sensing.

## 2 Simulation method

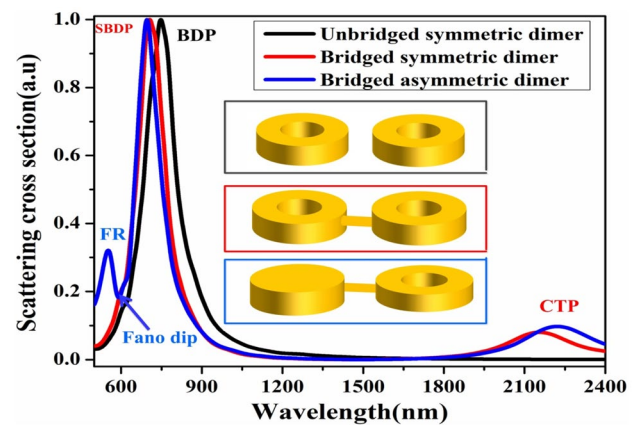
Figure 1 shows a schematic illustration of the studied nanoparticle (NP) dimers (bridged symmetric Au nanoring (NR) dimer and bridged shape-asymmetric Au nanoring-nanodisk (NR-ND) dimer in the present study. Initially, we used a bridged symmetrical Au nanoring (NR) dimer consisting of two identical nanorings each having an equal diameter ( $D = 100$  nm) and thickness ( $H = 50$  nm), and linked by a gold nanowire with a junction diameter ( $d = 10$  nm) and length ( $L = 20$  nm) suspended in a vacuum to explore the effect of symmetry breaking. Later, to explore the effect of the junction diameter and length on the optical responses of the bridged symmetric dimer (see



**Fig. 1** Schematic representation of the studied nanoparticle dimers. Graphic representation of bridged symmetric Au nanoring (NR) dimer (a) and bridged shape-asymmetric Au nanoring-nanodisk (NR-ND) dimer (b) with a diameter of  $D=100$  nm and thickness  $H=50$  nm, the dimers linked by a gold nanowire with the junction diameter ( $d=10$  nm) and length ( $L=20$  nm). The arrows in (b) exemplify the directions of the wave vector (blue) and polarization (red)

Fig. 1(a)) and the bridged shape-asymmetric dimer (see Fig. 1(b)), we varied the value of the junction diameter and length of the bridging nanowire. Finally, to investigate the sensing applications of CTP modes, the optimal bridged dimers were placed on a substrate with different refractive indices.

The bridged dimers were irradiated by a linear plane wave, which was injected along the  $z$ -axis, perpendicular to the plane of the nanosystems. As shown in Fig. 1(b), the polarization of the incident light was aligned along the dimer axis. The calculations of optical response of the bridged systems were carried out using the finite-difference time-domain (FDTD) method [31, 32], which solves Maxwell's equations by discretizing both time and space as well as by replacing derivatives with finite differences [33] to obtain the optical scattering spectrum. We used a total-field-scattered-field (TFSF) source, to calculate the optical responses of the studied nanostructure dimers that cover a spectral range from visible to mid-infrared (MIR) region (500–2500 nm). The dielectric functions of the designed systems were modeled using the experimental data of Johnson and Christy for gold [34]. To ensure the total absorption of electromagnetic radiation at the simulation boundaries we have used perfectly matched layer (PML) boundary conditions with layer of 64 layers in our simulations [5, 35] and the spatial grid sizes in all three axes were set to  $dx = dy = dz = 1$  nm. Additionally, simulation time step was set to the 300 fs according to the courant stability [36]. We used 2 nm mesh size in all  $x$ -,  $y$ -, and  $z$ - dimensions throughout the study. The convergence test of the calculation has been carried out, and the results



**Fig. 2** The spectral features of unbridged and bridged nanoparticle dimers. The black curve shows a scattering cross section of the bonding dimer plasmon (BDP) mode of the unbridged symmetrical Au NR dimer (see the black inset). The red curve displays, the SBDP and CTP that emerged in a bridged symmetric Au NR dimer (see the red inset). The blue curve displays the spectral spectrum of the Fano resonance (FR), the SBDP and CTP modes that emerge in the bridged shape-asymmetric Au NR-ND dimer (see the blue inset). In all three cases, the diameter of the nanoparticles was 100 nm

offered in the current study display that the error is within the satisfactory level [37, 38].

### 3 Results and discussion

#### 3.1 Effect of symmetry breaking on plasmonic modes of bridged nanodimers

Initially, for the direct comparison of the optical responses of symmetric Au NR dimer, the scattering spectra of bridged symmetric Au NR dimer and bridged shape-asymmetric Au NR-ND dimer are plotted together in Fig. 2. The symmetrical Au NR dimer allows for the excitation of classical dipolar mode due to the capacitive coupling [25]. Therefore, the scattering intensity of this dimer is dominated by the bonding dimer plasmon (BDP) mode at 750 nm [1], as shown by the black curve in Fig. 2. A bridged symmetrical dimer is connected with a conductive junction, the BDP mode blueshifts and forming the screened bonding dimer plasmon (SBDP) mode [16]. This is due to the junction screens parts of the local field at the gap. At the same time, a new resonance mode known as charge transfer plasmon (CTP) mode [10] emerges at a longer wavelength (lower frequency) in which the electron can directly flow between the two particles [16]. Thus, in bridged symmetric dimer with a conductive nanowire, the SBDP mode appeared at a shorter wavelength with high intensity [29] and a CTP mode appears at a longer wavelength with low intensity, as shown by the red curve in

Fig. 2. The position of SBDP mode of this dimer is located at 710 nm and its CTP mode is located at 2149 nm. The former is identified as a blueshifted bonding mode owing to a weaker polarization of the charge distribution of the individual nanoparticles and the later resonance mode is attributed to the electron density oscillates between the two particles, making one nanoparticle momentarily positively and the other negatively charged [39]. Due to the screening effect of the linking nanowire on plasmonic coupling, the SBDP mode of the bridged symmetric dimer shifts from 750 to 710 nm. The appearance of CTP modes at longer wavelengths is attributed to the flow of charges between two nanoparticles through bridging nanowires [24, 28]. In other words, the SBDP arises from constructive interference of transitions, whereas the CTP mode results from the destructive coupling of the same transitions at shorter separation distances. Moreover, due to constructive coupling, the SBDP mode produces a large intensity as predicted in the classical plasmon hybridization model, whereas the CTP mode has a lower intensity [40].

The spectral intensity of the bridged shape-asymmetric dimer displays three resonance modes, i.e., the SBDP peak with high intensity at 700 nm, the CTP peak with low intensity at 2233 nm and in addition to those peaks, a new Fano spectral shape (FR at 553 nm & Fano dip at 594 nm) is formed with low intensity (see Fig. 2 blue curve). As we discussed before, the resonance wavelength of the SBDP mode of this dimer tends to slight blueshift compared to the bridged symmetric dimer. The manifestation of the Fano spectral shape is ascribed to the destructive coupling of the bright and dark resonance modes of the system [35, 38]. Moreover, the FR and SBDP modes are in the visible region, whereas the CTP mode is in the mid-infrared (MIR) region. Furthermore, the resonance wavelength of CTP is redshifted approximately by about 84 nm and the amplitude of this mode became greater compared to the symmetric dimer (see red and blue curves in Fig. 2). This redshift can be ascribed to an increase in the charge separation distance of the bridged shape-asymmetric dimer, which results in a longer charge transport time and hence a lower CTP energy. Thus, the effect of broken symmetry on the plasmon couplings in bridged nanoparticle dimers gives additional freedom to tune and enhance the resonance wavelength and amplitude of the CTP feature, respectively. The main difference compared with the bridged symmetric dimer is the emerging of the Fano spectral shape. Due to the appearance of this FR mode, the tunability of the CTP mode and its improved intensity, the bridged shape-asymmetric dimer is found to be ideal for many applications, such as molecular sensing and building active nanodevices. In the next sections, we will discuss the effect of the junction diameter on enhancing

the tunability of charge transfer plasmon resonances in both bridged symmetric and shape-asymmetric systems.

### 3.2 The effects of nanowire junction geometries on the charge transfer plasmon modes of linked nanodimers

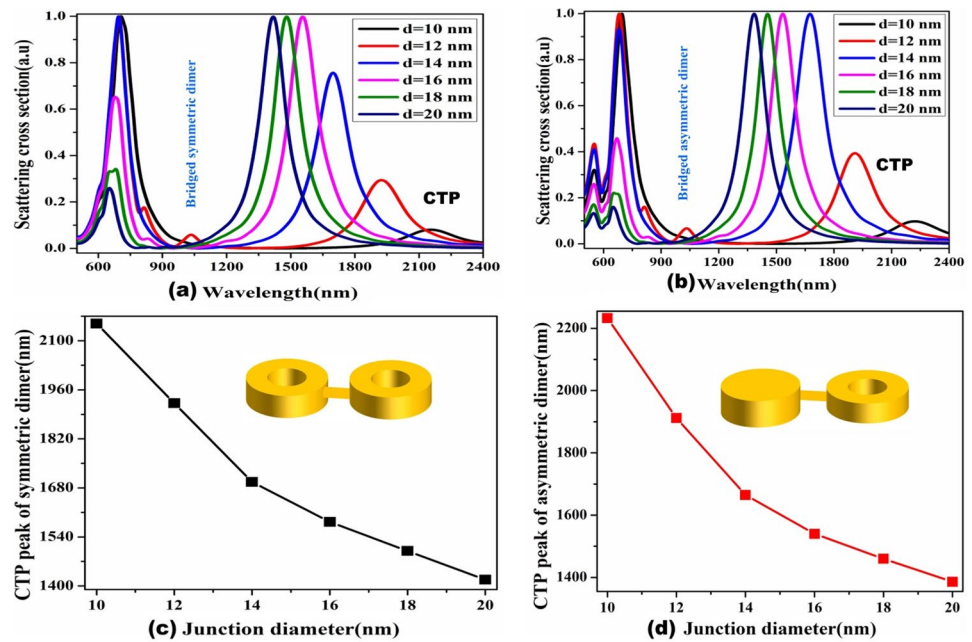
The CTP of bridged symmetric and shape-asymmetric dimers is extremely tunable mode that its resonance wavelength and intensity can be modified by monitoring the geometries of the bridging nanowire [5, 10, 15]. The conductance  $G$  of the linked nanowire is defined by the conductivity  $\sigma_j$  and geometric parameters including the length of the nanowire ( $L$ ) and the cross section of the contact area ( $A$ ) as follow [15]:

$$G = \sigma_j \frac{A}{L} \quad (1)$$

By keeping the overall length of the linking nanowire fixed, the effect of junction diameter on the tunability and enhancement of CTP spectral peaks is presented in Fig. 3. Figure 3(a & b) show the scattering cross section of bridged symmetric Au NR and shape-asymmetric Au NR-ND dimers as a function of the diameter of the bridging nanowire. Remarkable shifts and enhancement of the CTP mode are achieved by varying this parameter. The scattering spectra of both dimers with  $d = 10$  nm reveal that the CTP modes appear at 2149 nm and 2233 nm. The results show that increasing the junction diameter (from  $d = 10$  nm to 20 nm) leads to increasing the conductance, ensuing in a clear blueshift of CTP [10] and became narrower line width. Therefore, the CTP modes are blueshifted from 2149 to 1418 nm and 2233 nm to 1386 nm for bridged symmetric and shape-asymmetric dimers, respectively (see Fig. 3(c) and (d)). The changes in CTP resonances are approximately  $\Delta\lambda_{\text{CTP}} = 731$  nm and 847 nm, respectively. This is due to increasing the contact area leading to increased flow of charges and reduced time of charge transport between nanoparticles [10, 15]. Moreover, the blueshift of CTP with  $d$  ( $d = 2r$ ) may be instinctively implicit from a basic physical representation: when a certain quantity of charge  $Q$  transfers from one particle to another with an electric current  $I$ , the kinetic energy of CTP is approximately  $E_k = \frac{m_e L Q I^2}{2 n_0 e^2 \pi r^2}$ , where  $L$  is the effective distance between the center of transferred charge [12]. However, the effect of the junction diameter on the SBDP peak is insignificant compared to that of the CTP resonance peak. Moreover, the CTP modes in the bridged shape-asymmetric dimer can be adjusted with a high degree of freedom by changing the junction geometry compared to the bridged symmetric dimer. This substantial tunability of CTP mode makes shape-asymmetric dimer more attractive



**Fig. 3** (a) and (b) show the scattering cross section of the nanowire bridged symmetric dimer and shape-asymmetric Au NR-ND dimer as a function of junction diameter, respectively. (c) and (d) CTP peak positions for bridged symmetric and shape-asymmetric dimers as a function of the junction diameter, respectively



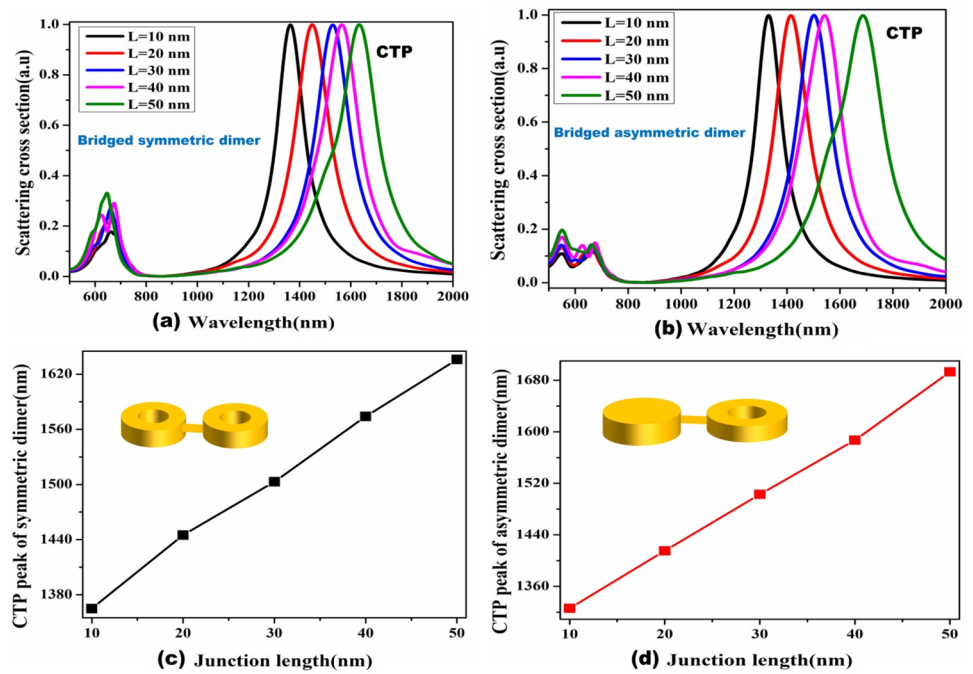
in practical applications such as molecular sensing and building active nanodevices [24].

The intensity of the CTP modes is strongly dependent on the diameter of a bridged nanowire. Moreover, the amplitude of these modes progressively increases with increasing the junction diameter, while the intensity of the SBDP mode concurrently decreases, as shown in Fig. 3(a) & (b). Furthermore, due to the high conductance tendency and improved screening effect, the intensity of the CTP mode is increased significantly [15]. Thus, the spectral width and resonance wavelength of this mode in bridged dimers can be easily manipulated by controlling the junction geometries [5]. The CTP mode is inversely proportional to the junction diameter (see Fig. 3(c) & (d)). Our results disclose that the effect of junction diameter on the spectral behavior of CTP in bridged asymmetric dimer is significant compared to the bridged symmetric dimer.

As shown above, by varying the conductivity and geometric parameters of the nano bridge, it is possible to modify the resonance wavelength of CTP modes in bridged nanoparticle dimers [15, 29]. Here, we further strengthen this fact by investigating the effect of junction length on the spectral properties of CTP modes of linked symmetric and asymmetric nanodimers with fixed nanowire cross section. The diameter of nanoparticles in both dimers is  $D_1 = D_2 = 100$  nm, and the diameter of the nanowires in the junction is kept constant ( $d = 20$  nm), while the length of the junction ( $L$ ) is increased from 10 to 50 nm. The CTP spectra in the near-infrared and mid-infrared regions were recorded. Figure 4 displays the calculated scattering cross-sections of bridged symmetric Au NR and shape-asymmetric Au NR-ND dimers for different junction lengths. The resonance wavelengths of the CTP

modes of the former and the latter dimers with  $L = 10$  nm are 1365 nm and 1326 nm, respectively (see Fig. 4(a) & (b) black curves). It is found that the CTP modes can be tuned from 1365 to 1636 nm and 1326 nm to 1693 nm wavelength, respectively with increasing junction length from  $L = 10$  nm to  $L = 50$  nm (see Fig. 4(c) & (d)). As one increases the junction length, the changes in the CTP modes of bridged symmetric dimer and shape-asymmetric dimer are approximately  $\Delta\lambda_{\text{CTP}} = 271$  nm and 367 nm, respectively. This significant shift of the CTP mode is due to the weak restoring force between the oscillating charges on the two nanoparticles [12]. Moreover, an increase in the junction length increases the charge transport time, giving rise to a lower CTP resonance energy of the system. This mode can be changed from the NIR to the MIR regime, by increasing the junction length [24]. The magnitude of the redshift depends on the time needed for the electrons to cross the junction, which is inversely proportional to the conductance [6]. Here, the remarkable redshift in the position of the CTP mode can be interpreted in terms of the charge transport time, which is also closely related to the junction length. It was shown that increasing the junction length leads to a longer time and lengthier path for traveling the induced charges across the junction, resulting in a significant reduction in the quality of the CTPs [25]. Moreover, by changing the geometries of the nanojunction, one can tune the resonance wavelength of CTP in bridged dimers [15]. Compared to symmetric dimers, the tunability of the resonance wavelength of CTP modes in the shape-asymmetric dimer is very significant. Furthermore, these properties make the CTP modes in the asymmetric dimer suitable candidates for molecular sensing and building active nanodevices.

**Fig. 4** (a) and (b) show the scattering cross-sections of the nanowire bridged symmetric dimer and shape-asymmetric Au NR-ND dimer as a function of junction length, respectively. (c) and (d) CTP peak positions for bridged symmetric and shape-asymmetric dimers as a function of the junction length, respectively

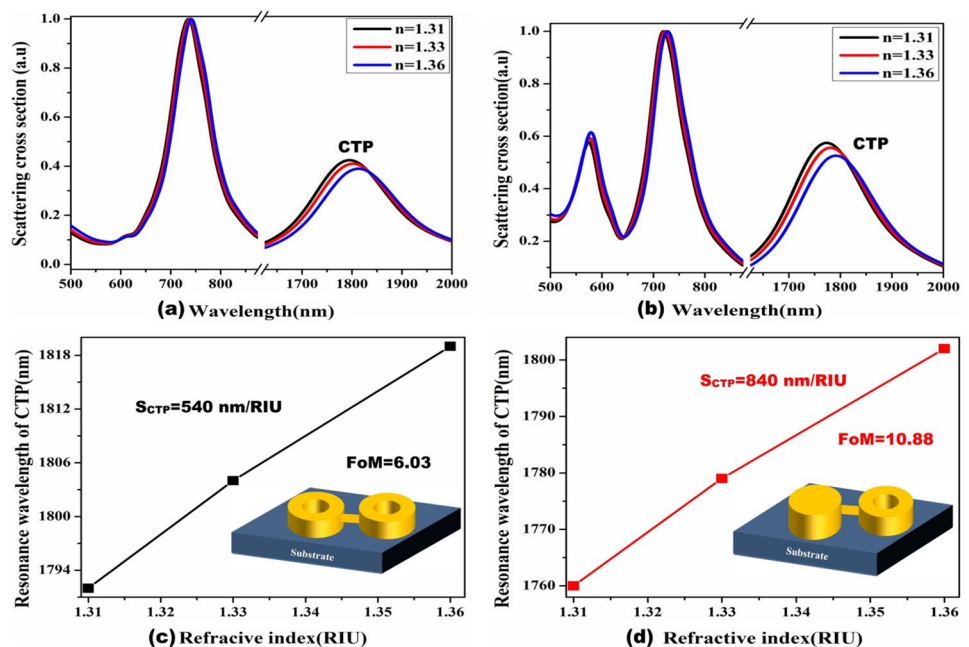


### 3.3 Sensing application of charge transfer plasmons

The CTP mode in bridged nanoparticle dimers has great potential applications in sensing [15] due to the substantial tunability of its wavelength through the geometry of a linking nanowire. Here, we used optimal bridged symmetric Au NR and shape-asymmetric Au NR-ND dimers to calculate the sensing performance of the CTP modes with a fixed

diameter and length of the linked nanowire in the detection of refractive indices of the substrate as shown in the inset of Fig. 5(c & d). The key parameters used to evaluate the sensor performance are sensitivity and FoM [41]. More recently, there has been growing interest in this kind of study using Fano resonances [35, 38, 42], because of the sharp spectral features [29]. In this section, we have explored the sensitivity of CTP modes in bridged dimers as a function of the refractive index of the substrate.

**Fig. 5** Sensitivity of bridged symmetric and asymmetric dimers as a function of the refractive index of the substrate. (a) and (b) show the calculated normalized scattering spectra of bridged symmetric and shape-asymmetric dimers with the junction diameter ( $d=14$  nm) and length ( $L=20$  nm) as a function of the refractive indices. (c) and (d) Linear plot of CTP peak shifts of symmetric and asymmetric dimers as a function of the refractive indices of the substrate



The sensing abilities of bridged symmetric Au NR and shape-asymmetric Au NR-ND dimers as a function of the refractive index of the surrounding medium for fixed junction diameter ( $d = 14$  nm) and junction length ( $L = 20$  nm) are presented in Fig. 5(a) & (b). The other geometrical parameters are the same as those used in the previous sections. The resonance wavelengths of the CTP modes in bridged symmetric and shape-asymmetric dimers with a refractive index of 1.31 are 1792 nm and 1760 nm, respectively, as shown in the black curves in Fig. 5(a) & (b). The CTP mode exhibit a redshift from 1792 to 1819 nm and 1760 nm to 1802 nm, as the refractive index increases to 1.36, as shown in the blue curves in Fig. 5(a) & (b). Therefore, the resonance wavelength shifts in these modes by varying the refractive index of the environment from 1.31 to 1.36 are found to be 27 nm and 42 nm, respectively (see Fig. 5(c) & (d)). It is evident from Fig. 5(a) and (b) that, the tunability of CTP mode in bridged shape-asymmetric dimer is more significant compared to bridged symmetric dimer as the refractive index of the substrate increases. Hence, it is recommendable that the CTP mode in bridged asymmetric dimers is suitable for real-world applications instead of the more commonly used bridged symmetric dimers.

The sensitivity of metallic nanoparticle dimers is extremely dependent on the refractive index of the surrounding media [35, 38, 43]. Here, the sensitivity ( $S$ ) of the CTP mode is given as the change in this mode per change in refractive index ( $S = \Delta\lambda_{CTP}/\Delta n$ ) and, it is measured in nm per refractive index unit (RIU) [38, 43]. Therefore, the sensitivities of CTP modes in bridged symmetric and shape-asymmetric dimers are approximately 540 nm/RIU and 840 nm/RIU, as shown in Fig. 5(c) & (d), respectively. This indicates that the bridged shape-asymmetric dimer has better sensitivity than the bridged symmetric dimer. These large sensitivities are mainly due to the significant shift of the CTP modes that occur when varying the refractive index of the surrounding medium. Compared to the sensitivity obtained from Fano resonance [35, 38], these largest values  $S_{CTP}$  attained by the significant shifts of the CTP modes make bridged dimers good candidates for standard LSPR shift-based sensing [15]. FoM is a key factor that is widely used to assess the performance of CTP modes in bridged nanoparticle dimers [15]. The efficiency of CTP in bridged dimers is typically assessed by its FoM, defined as [29, 44]:

$$FoM = \frac{S_{CTP}}{FWHM} \quad (2)$$

where  $S_{CTP}$  is the linear slope for the refractive index dependence, that is, the ratio of the CTP resonance wavelength shift to the change in the refractive index of the surrounding medium, and FWHM is the full width at half maximum of the resonance mode. Hence, using Eq. (2) the

values of FoM calculated for the CTP modes of bridged symmetric and shape-asymmetric dimers are 6.03 and 10.88, respectively. A comparable result was reported by Perez-Gonzalez et al. for a strongly coupled nanoparticle dimer linked by a molecular junction [44]. Due to the substantial tunability of the CTP resonance mode through the refractive index of the surrounding medium, the value of FoM for the bridged asymmetric dimer is found to be larger than that of a bridged symmetric dimer. Using the Fano resonances, the largest FoM values have been achieved in the literature, on the order of 10–20 [45]. Thus, the CTP modes in bridged nanoparticle dimers are the best candidate for normal LSPR based sensing [44]. This result provides a good opportunity to sense CTP resonance modes and increases its application potential for molecular sensing.

## 4 Conclusions

In summary, we have explored the tunability of the CTPs of bridged symmetric and shape-asymmetric dimers through varying the geometries of the bridging nanowire and refractive index of the substrate using the finite-difference time-domain methods. Varying the junction diameter and length of the bridging nanowire controls the resonance wavelengths and scattering spectra of the CTP modes. Increasing the diameter (length) of nanowire shifts CTP modes to considerably shorter (longer) wavelengths in the near and mid-infrared regions of the spectra. Moreover, the position of these modes mainly depends on the junction geometries and the refractive index of the substrate, which will be useful for applications in molecular sensing. Similarly, the intensity of CTP mode can be modified by varying the aforementioned parameters. Lastly, we explored the bulk sensing applications of CTP with optimized geometries to evaluate the ability of this mode in the detection of change in refractive index of a substrate. Hence, we expect that our result is significantly important in designing tunable nanodevices in near and mid-infrared regions for practical applications in nanomotors, sensing and other optoelectronic devices.

**Data availability** The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

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