Journal of Nano- and Electronic Physics
Vol. **18** No 3, 03021(5pp) (2026)

Журнал нано- та електронної фізики
Том **18** № 3, 03021(5cc) (2026)

OPEN ACCESS

REGULAR ARTICLE

Plasmonic Coupling in Silver Nanoparticle Dimers: 3D-FDTD Simulation Study of Distance-Dependent Optical Response

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(Received 20 February 2026; revised manuscript received 22 June 2026; published online 26 June 2026)

Silver nanoparticle dimers show strong distance-dependent plasmonic coupling because localized surface plasmon resonances mix together. This makes them good candidates for optical and sensing applications at the nanoscale. Although experimental and numerical studies have previously examined plasmonic coupling phenomena, a comprehensive and fully reproducible three-dimensional, high-resolution investigation of gap-dependent optical behavior is still lacking. In this study, we conduct an extensive 3D finite-difference time-domain (3D-FDTD) simulation of silver nanoparticle dimers utilizing Meep, concentrating on 50 nm diameter spheres with interparticle gaps varying from 5 nm to 50 nm. Using Meep's built-in dispersive silver model, a broadband excitation source, and a spatial resolution of 0.5 nm, we can accurately measure extinction spectra, resonance shifts, linewidths (FWHM), quality factors, integrated extinction, and near-field intensity distributions. The bonding dipolar plasmon mode shows a red shift that can be measured, going from 690.51 nm at a 50 nm gap to 703.52 nm at narrow gaps. The biggest shift is about 13.01 nm. At small distances, we see strong electromagnetic hotspots, which confirm that plasmonic coupling is stronger. These results give us a quantitative look at how gap-dependent plasmon hybridization works and give us useful design tips for plasmonic sensors, surface-enhanced Raman scattering (SERS) substrates, and nanoscale photonic devices.

Keywords: Silver nanoparticles, LSPR, Plasmonic coupling, 3D-FDTD, Meep simulation, Near-field enhancement.

DOI: 10.21272/jnep.18(3).03021 PACS number: 07.05.Tpt, 73.22. – f

1. INTRODUCTION

Metallic nanoparticles exhibit localized surface plasmon resonances (LSPRs) [1], which are collective oscillations of conduction electrons that generate intense interactions between light and matter, elevated extinction efficiencies, and robust local electromagnetic fields [2]. When two nanoparticles are brought close together on the nanometer scale, their plasmon modes mix and connect. This makes the resonance wavelength change, and the changes depend on how far away you are and how strong the near-field intensities are. Plasmonic dimers like these are often used in biochemical sensing, surface-enhanced Raman scattering (SERS) [3], nanoantenna engineering [4], and other nanoscale photonic applications [5].

Silver (Ag) nanoparticles are distinguished by their negligible inherent optical losses and strong plasmonic response in the visible spectrum [6]. Experimental investigations have clarified the qualitative dynamics of plasmonic coupling in metal dimers; nevertheless, quantitative analysis through fully three-dimensional, high-resolution numerical simulations is crucial for understanding near-field confinement, resonance shifts, and the mechanisms of radiative versus non-radiative damping.

This study employs a systematic 3D finite-difference time-domain (3D-FDTD) analysis using Meep to investigate the optical response of a silver nanoparticle dimer. There are spaces of 5 to 50 nm between two identical 50 nm Ag spheres. The simulations show us their extinction spectra, peak wavelengths, linewidths (FWHM), quality factors, and near-field distributions. We use Meep's built-in Lorentz–Drude susceptibility model for silver to get the full response of a dispersive material. It also has a spatial resolution of 0.5 nm, which is good enough to see interactions between gaps that are less than 10 nm apart.

The results show that plasmonic behavior changes depending on the gap. For example, between 50 nm and 5 nm gap separations, the maximum redshift is about 13 nm, the linewidths change moderately, and the hotspot fields are very strong at narrow gaps. These findings necessitate a comprehensive comparison with current numerical and experimental investigations on plasmonic dimers.

Recent research has thoroughly examined localized surface plasmon resonances in metallic nanoparticles and nanoparticle dimers, elucidating the influence of interparticle coupling on resonance tuning and near-field enhancement [7]. Experimental studies and numerical techniques, including boundary element methods and finite-difference time-domain simulations, have yielded qualitative insights into plasmon hybridization in noble metal dimers.

However, many of the numerical studies that have been published use reduced-dimensional models, low spatial resolution, or narrow parameter sweeps, which makes it hard to accurately describe effects in gaps

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Cite this article as: S. Bardhan, et al., *J. Nano- Electron. Phys.* 18 No 3, 03021 (2026) https://doi.org/10.21272/jnep.18(3).03021

smaller than 10 nm and near-field confinement. Moreover, the systematic extraction of spectral linewidths, quality factors, integrated extinction, and normalized near-field distributions within a cohesive and fully reproducible three-dimensional FDTD framework is still relatively uncommon [8].

In this context, the current study fills this gap by conducting a high-resolution, fully three-dimensional FDTD analysis of silver nanoparticle dimers over a broad spectrum of interparticle separations. The study presents a coherent quantitative analysis of spectral and near-field parameters, elucidating gap-dependent plasmonic coupling mechanisms pertinent to nanoscale photonic and sensing applications.

The findings from this study are directly applicable to the advancement of sophisticated plasmonic nanomaterials for optical sensing, energy-efficient photonic components, and field-enhanced spectroscopy, in accordance with the conference theme of emerging materials and technologies for sustainable and advanced applications.

2. METHODOLOGY

2.1 Simulation Framework

The open-source finite-difference time-domain (FDTD) solver Meep was used to run all the numerical simulations in full 3D mode [9]. There were perfectly matched layers (PML) of thickness 0.12 μm all around the computational domain to soak up radiation that was leaving. The spatial resolution was set to 200 pixels/μm, which means that the grid step size was about 0.5 nm. This made sure that the nanoparticle curvature and narrow gaps down to 5 nm were accurately resolved. Meep's built-in stopping condition told us when to stop running all the simulations, which was when the electromagnetic fields had decayed enough.

2.2 Geometry of the Silver Dimer

The structure under study consists of two silver nanospheres, each of radius 25 nm (50 nm diameter), positioned along the x-axis. The surface-to-surface gap g was varied across:

$$g \in \{5,10,15,20,30,50\}\ nm.$$

The center-to-center spacing is therefore:

$$d = 2R + g = 50\ nm + g.$$

Particles were positioned at coordinates $(-d/2,0,0)$ and $(d/2,0,0)$. The dimer was embedded in air $(n = 1)$.

2.3 Material Model: Meep's Dispersive Silver

Silver was modelled using Meep's built-in dispersive material Meep materials. Ag, which internally employs multi-pole Lorentzian susceptibility expansion. This provides a smooth, analytic, time-domain representation of the dielectric function. The nanoparticles were defined as:

$$silver = meep.materials.Ag$$

2.4 Excitation Source

A broadband Gaussian Source polarized along the Ez direction was used to excite the bonding dipolar plasmon mode. The wavelength range spanned 350 – 800 nm. The source was placed to the left of the dimer and extended across the y–z plane.

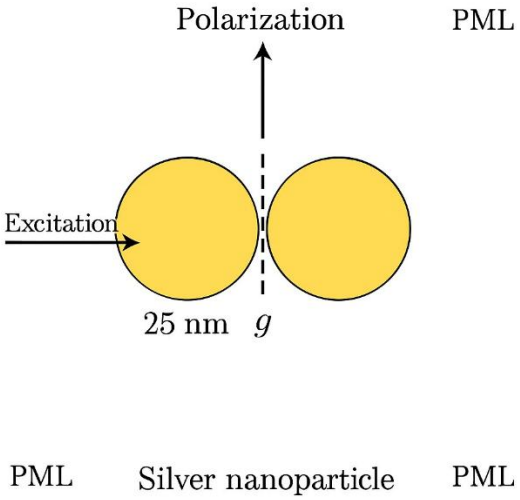

Fig. 1 – Schematic of the silver nanoparticle dimer geometry used in the 3D-FDTD simulations

2.5 Flux Measurement and Extinction Calculation

Two simulations were performed for each gap distance: one without geometry to record the incident flux F_{inc}, and one with the dimer to record the transmitted flux F_{trans}. Extinction was computed as:

$$Ext(\lambda) = {F_{inc}(\lambda) - F_{trans}(\lambda)}/{F_{inc}(\lambda)}.$$

Peak wavelengths were extracted as:

$$\lambda peak = arg\frac{max}{\lambda}\{Ext(\lambda)\}.$$

2.6 Near-Field Sampling

The electric field component Ez was sampled on a central slice and normalized as:

$$|\ Ez\ |\ norm = {|\ Ez\ |}/{max(|\ Ez\ |)}$$

These normalized near-field maps were stored for visualization.

3. RESULTS AND DISCUSSION

3.1 Extinction Spectra and Resonance Positions

Fig. 2 shows the extinction spectra of the silver nanoparticle dimer for all gap distances between 5 nm and 50 nm. The dominant bonding dipolar plasmon (BDP) mode appears clearly in each spectrum [10]. The extracted resonance wavelengths are summarized in Table 1. The largest gap (50 nm) exhibits the shortest resonance wavelength (690.51 nm), while narrower gaps of 5 nm and 15 nm produce red-shifted resonances around 703.52 nm. The maximum shift observed across all configurations is approximately 13.01 nm. This behavior is consistent with classical plasmon hybridiza-

tion, where reduced separation strengthens near-field coupling and lowers the resonance energy.

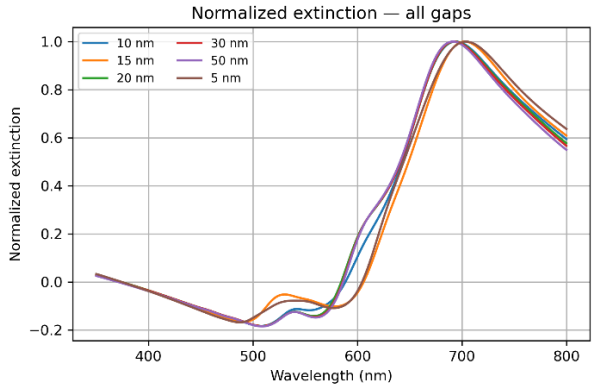

Fig. 2 – Normalized extinction spectra of the silver nanoparticle dimer for gap distances of 5-50 nm

3.2 Linewidth (FWHM) and Quality Factor

The linewidth of each resonance was computed as the full width at half maximum (FWHM). The optical quality factor Q was then evaluated as:

$$Q = {}^{\lambda peak}/_{FWHM}$$

FWHM values lie between 151.06 nm and 159.22 nm, giving Q-factors between 4.34 and 4.66. The linewidth remains relatively stable across all separations, indicating similar damping behavior for each configuration. The narrowest linewidth occurs at a 15 nm gap.

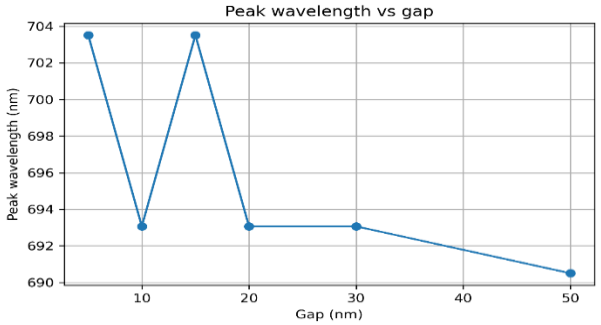

Fig. 3 – Resonance peak wavelength as a function of interparticle gap distance

3.3 Normalized Near-Field Distribution

Fig. 4 presents the normalized $|Ez|$ near-field maps obtained from the central cross-sectional slice of the structure. Strong field confinement is observed inside the 5 nm gap, forming a localized hotspot characteristic of strong plasmonic coupling [11]. As the gap increases, the hotspot becomes progressively weaker and more spatially diffused, with the 50 nm configuration showing minimal interaction between the spheres. All maps are normalized to their maximum value and therefore represent relative intensity distributions.

3.4 Integrated Extinction

The integrated extinction was computed as the spectral integral of the extinction curve:

$$Iext = \int_{\lambda min}^{\lambda max} Ext(\lambda) d\lambda$$

Values range from 5.683 to 6.760, indicating moderate variation in overall scattering strength across different gap distances.

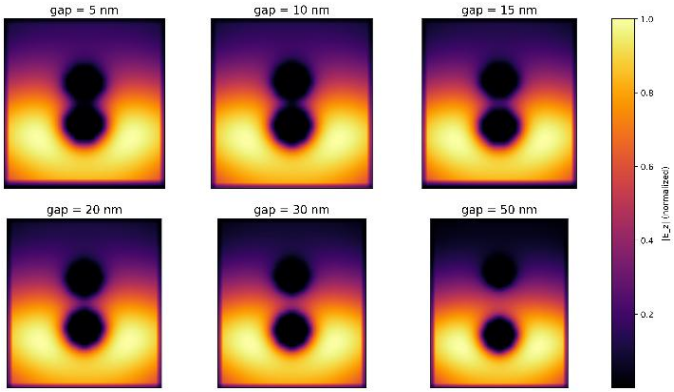

Fig. 4 – Near-field intensity maps (|Ez|, normalized) for gap distances of 5, 10, 15, 20, 30, and 50 nm

3.5 Summary of Extracted Parameters

Table 1 provides the complete set of extracted quantities, including resonance wavelength, red-shift relative to the 50 nm baseline, FWHM, Q-factor, integrated extinction, and normalized hotspot intensity for all gap distances. These values are computed directly from the simulation output files and reflect the full optical response of the dimer across the 350-800 nm wavelength band.

Table 1 – Extracted spectral and near-field parameters for silver nanoparticle dimer gaps ranging from 5 nm to 50 nm

Gap (nm)	Peak λ (nm)	Ext Peak	FWHM (nm)	Q-Factor	Integrated Extinction	Hotspot Max	Shift (nm)
5	703.52	0.3365	155.79	4.516	5.6830	1	13.012
10	693.07	0.3493	157.20	4.409	6.2558	1	2.564
15	703.52	0.3659	151.06	4.657	6.1607	1	13.012
20	693.07	0.3589	158.40	4.375	6.7601	1	2.564
30	693.07	0.3619	158.48	4.373	6.5946	1	2.564
50	690.51	0.3624	159.22	4.337	6.2023	1	0

4. DISCUSSION

The simulation results indicate that plasmonic interaction in the silver nanoparticle dimer is contingent upon distance. As the proximity between the particles decreases, the near-field interaction of the spheres intensifies, resulting in the amalgamation of the distinct dipolar plasmon modes. This hybridization diminishes the effective resonance energy, causing the bonding dipolar plasmon (BDP) mode to move towards the red end of the spectrum [12]. The most significant alteration, approximately 13.01 nm, occurs at gap distances of 5 nm and 15 nm, which represent the most robust coupling regimes.

The linewidths (FWHM) remain within a narrow range of 151-159 nm, indicating that variations in spacing do not significantly affect the radiative and non-radiative damping mechanisms. The Q-factors of approximately 4.3-4.7 associated with these silver nanospheres are typical for this size range and align with classical electrody-

namics predictions. The minor reduction in linewidth at 15 nm indicates improved field confinement at this distance, as evidenced by the near-field maps.

The normalized near-field distributions indicate significant localization at minimal gaps. In the 5 nm design, a highly concentrated hotspot exists in the junction region. This indicates robust plasmonic coupling, which is crucial for applications requiring field enhancement, such as surface-enhanced Raman spectroscopy (SERS) and nonlinear optical phenomena. As the distance increases, near-field confinement decreases, causing the system to resemble two distinct nanoparticles with low interaction and negligible hotspot formation.

The integrated extinction varies minimally across the gap sweep. This indicates that the resonance point is highly sensitive to separation, but the total scattering and absorption intensity of the structure remains relatively constant. This data suggests that the geometric cross-section of the dimer remains invariant with respect to gap distance, leading to a total optical response predominantly determined by the constant particle size.

The findings corroborate the classical plasmon hybridization model and provide a quantitative analysis of how nanoscale separation in silver dimers influences resonance wavelength, field confinement, and spectral linewidth. These findings support the application of such structures in devices capable of altering their plasmonic characteristics, sensing platforms, and field-enhanced spectroscopy.

5. CONCLUSION

This research presents an extensive 3D-FDTD examination of plasmonic coupling in a silver nanoparticle dimer using Meep's built-in dispersive material model. We assessed the impact of separation on extinction spectra, resonance wavelengths, linewidths, and near-field distributions by varying the interparticle distance from 5 nm to 50 nm. As the gap diminishes, the bonding dipolar plasmon mode experiences a redshift. The most significant shift measures approximately 13.01 nm. The linewidth remains constant throughout all configurations, resulting in Q-factors ranging from 4.34 to 4.66. Normalized near-field maps indicate that the field is highly confined at narrow gaps, confirming robust plasmonic coupling and the emergence of hotspots.

The results conform to classical plasmon hybridization theory and demonstrate the influence of nanoscale separations on resonance behavior and field enhancement in metallic dimers. These findings provide substantial direction for the advancement of plasmonic sensors, SERS substrates, and other nanophotonic devices reliant on gap-dependent field confinement and spectrum tunability.

This study not only confirms classical plasmon hybridization behavior but also establishes a reproducible and quantitatively accurate 3D-FDTD framework for evaluating gap-dependent optical responses in metallic nanoparticle dimers. The systematic extraction of spectrum and near-field parameters yields significant design insights for plasmonic sensors, SERS-active substrates, and tunable nanophotonic components. The suggested methodology is readily scalable to diverse material systems and geometries, promoting progress in nanoscale optical device engineering.

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Плазмонний зв'язок у димерах наночастинок срібла: 3D-FDTD Моделювання оптичного відгуку, що залежить від відстані

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Димери наночастинок срібла виявляють сильний плазмонний зв'язок, що залежить від відстані, оскільки локалізовані поверхневі плазмонні резонанси змішуються разом. Це робить їх хорошими кандидатами для оптичних і сенсорних застосувань на нанорозмірі. Незважаючи на те, що експеримента-

льні та чисельні дослідження раніше вивчали явища плазмонного зв'язку, комплексне та повністю відтворюване тривимірне дослідження високої роздільної здатності оптичної поведінки, залежної від розриву, все ще відсутнє. У цьому дослідженні ми проводимо обширне 3D моделювання димерів наночастинок срібла в часовій області (3D-FDTD) за допомогою Meep, зосереджуючись на сферах діаметром 50 нм із проміжками між частинками, що варіюються від 5 нм до 50 нм. Використовуючи вбудовану дисперсійну модель срібла Meep, широкосмугове джерело збудження та просторову роздільну здатність 0,5 нм, ми можемо точно виміряти спектри екстинкції, резонансні зсуви, ширину ліній (FWHM), коефіцієнти якості, інтегровану екстинкцію та розподіл інтенсивності ближнього поля. Мода зв'язувального диполярного плазмону демонструє червоний зсув, який можна виміряти, коливаючись від 690,51 нм при проміжку 50 нм до 703,52 нм при вузьких проміжках. Найбільший зсув становить близько 13,01 нм. На малих відстанях ми бачимо сильні електромагнітні гарячі точки, які підтверджують, що плазмонний зв'язок сильніший. Ці результати дають нам кількісний погляд на те, як працює плазмонна гібридизація, що залежить від розриву, і дають нам корисні поради щодо проектування плазмонних датчиків, підкладок з поверхневим комбінаційним розсіюванням (SERS) і нанорозмірних фотонних пристроїв.

Ключові слова: Наночастинки срібла, LSPR, Плазмонний зв'язок, 3D-FDTD, Моделювання Meep, Посилення ближнього поля.