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Anisotropic optical response of gold-silver alloys

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ABSTRACT

Gold and silver alloys enable novel opportunities for engineering materials with distinct optical responses. Here we investigate the optical properties of gold and silver ($\text{Ag}_x\text{Au}_{1-x}$) structures using First-Principle Density Functional Theory (DFT) for gold concentrations varying from 0% up to 100% with steps of 25%. Results of the optical permittivity are analyzed with the independent particle approximation and compared with previously reported theoretical and experimental works. The pure systems and the ones with unbalanced concentrations exhibit isotropic optical responses. The $\text{Ag}_{0.50}\text{Au}_{0.50}$ shows an anisotropic response among the y-direction and the xz-direction, mainly in the intraband transition energy range. The anisotropy is elucidated in terms of the d-orbitals density of states and the charge distribution with the structure. The anisotropic optical response can be the origin of the discrepancies among reported experimental results for structures with the same stoichiometry.

Introduction

Alloying in photonics is a promising route for obtaining materials properties and functionalities otherwise unachievable with single material-based structures¹⁻⁴. Combining different chemical elements opens up avenues of possibilities to fine-tune the optical and electronic response of devices for a broad range of applications such as energy harvesting⁵, continuous-wave and pulsed lasing^{3,6}, and non-linear optics⁷. In the last decade, the rapid progress of the plasmonic field occurred due to the advance of new techniques of fabrication and characterization of pure metallic structures^{4,8}. More recently, a change

of paradigm driven by the maturing of nanofabrication methods and the systematic analysis of alloyed nanostructured systems^{9–11} resulted in the rise of applications of this novel system as plasmonic tweezers¹², hydrogen sensors¹³, photocatalysts¹⁴, and bio-sensors¹⁵.

The complex permittivity of materials is directly related to their optical properties. The control of the permittivity through alloying allowed the engineering of surface plasmon polariton (SPP) resonances, diversifying and increasing the efficiency of devices such as sensors, nanoscale lasers, and solar cells^{10, 16, 17}. For pure metals, the permittivity is well described in the literature. However, for alloys, there is a lack of fundamental knowledge and agreement about the physical processes underlying their optical response⁴. To predict the permittivity of a certain compositions, theoretical approaches employed linear interpolation between the alloy's counterparts. Nevertheless, especially for noble metals, there was no good agreement with experiments, leading to spurious effects as negative absorptions¹⁸. This is mainly due to complex mechanisms such as band hybridization¹⁹. Also, effective multi-parametric Drude-Lorentz-like models were used to fit experimental results, accounting for frequency-dependent corrections of interband transitions^{9, 18, 20, 21}. Here, there was no consensus among fitted parameters, leading to differences in the description of the visible and near ultra-violet optical responses⁹. Finally, in a parameter-less fashion, ab-initio methods such as the density functional theory (DFT) were used to elucidate several aspects of the optical properties of alloys^{4, 21, 22}. The advantage of using computational approaches lies in the fact that it is a much faster route to predict materials properties than the traditional fabrication and measurement methods. This has lead to unprecedented development in materials discovery^{4, 23}. The possibilities of combining materials and properties are numerous, and there are always unexplored aspects of it.

From the optical point of view, materials with unique properties can lead to applications that explore new degrees of freedom for optical processes. That is the case of birefringent materials, whose response depends on the polarization of the incident light, with applications as optical waveguide-polarizers with exceptional extinction ratios^{24, 25}. At the nanoscale, new degrees of freedom in the optical response can be achieved by manipulating the localized surface plasmon polariton (LSP) via the shape and/or size of nanoparticles²⁶, nanorods^{27, 28}, nanowires²⁹, and ultrathin metal films³⁰. Particles with different shapes lead to anisotropic linear optical responses^{26, 29, 30}. Anisotropic non-linear properties also play a meaningful contribution due to their dependence on the shape of the nanostructure^{26, 31}. However, we

believe the analysis of the anisotropic optical behavior of bulk alloys is still underestimated and should receive prior attention to the nanostructured systems.

In this work, we report on the application of DFT to obtain the bulk permittivity of gold and silver alloys with concentrations ranging from the pure metals to 25% Au (75% Ag), 50% Au (50% Ag), and 75% Au (25% Ag). For the $\text{Ag}_{0.50}\text{Au}_{0.50}$ alloy, we show that the optical response is anisotropic due to an unbalanced charge distribution among the Au and Ag atoms. Using DFT with the Generalized-Gradient-Approximation (GGA) exchange-correlation functional, we calculate the influence of stoichiometry on the band structures, the density of states, and the energy-dependent permittivity with the independent particle approximation²³. We observe a drastic difference between the y -direction and the xz -direction of the permittivity in the intraband energy regime. The intraband transitions are heavily dependent on the shape of the d -orbitals in the valence band. Here, we confirm that the d_{xz} orbital differs from the d_{xy} and d_{yz} due to an unbalanced charge distribution in the structure. For all other chemical compositions, the optical response is isotropic, as expected for a cubic periodic unit cell.

Results and Discussion

Band Structure and Density of States

To obtain the permittivity of the Ag-Au alloyed structures, we first perform their structural relaxation and calculate their band structures using the Quantum ESPRESSO package³² (See the Methods section for further computational details). Figs. 1(a)-(e) shows the unit cells of the five metallic structures (Ag, $\text{Ag}_{0.75}\text{Au}_{0.25}$, $\text{Ag}_{0.50}\text{Au}_{0.50}$, and $\text{Ag}_{0.25}\text{Au}_{0.75}$, and Au, respectively) used in our calculations. All compositions have a face-centered-cubic crystal structure. We perform DFT calculations of the relaxed structures with the GGA and the Perdew–Burke–Ernzerhof (PBE) parameterization, accounting for relativistic effects through the Hamann optimized scalar-relativistic norm-conserving pseudopotential (See the Methods section for further computational details). Figs. 1(f)-(j) presents the calculated band structure. As expected, all systems have the absence of the band gap encompassing the Fermi-Level, characteristic metals, with a continuous transition of the electronic response from pure Ag to pure Au²¹. The projected density of states (DOS) are displayed in Figs. 1(k)-(o). The predominance of d -orbitals in the valence band hybridized with the s -orbitals ensures the transition metal characteristic of all structures. For Ag,

Figure 1. Density functional theory (DFT) calculations of $\text{Ag}_x\text{Au}_{1-x}$ structures. (a)-(e) Schematics of the face centered cubic unitary cells. (f)-(j) Band structure calculations showing empty states (> 0 eV) and the d-bands (< 0 eV). (k)-(o) Calculated density of states (DOS) with total (black line) and projected density of states (PDOS) for the s - (red), p - (green), and d -orbitals. The transition metal character of both Au and Ag structures is also observed in the alloys. This is characterized by the predominance of the d orbital (light-gray line) contribution to the DOS.

the intraband transitions are mainly governed by the energy range between -6 eV to -3 eV that bounds the majority of d -orbitals (Fig. 1(k)). Increasing the Au concentration a broaden in energy towards the Fermi-Level is observed due to relativistic effects related to the a bigger atomic mass of Au in comparison to Ag (Figs. 1(l)-(n))³³. The scalar-relativistic contribution to the valence band (namely, the mass-velocity and the Darwin terms) lowers the s -orbitals energy stabilizing them and shielding the nuclei^{34,35}. The latter shifts the d -orbitals towards the Fermi-Level (Figs. 1(k)-(o) and Fig. S1), resulting in the expected optical response of Au³⁶. The contribution of relativistic effects to the conduction band occurs only for f -orbitals, having low contribution on the energy range of transitions analysed. Likewise, for the valence band, we observe a band split of order of 10^{-3} eV with no significant impact on the optical properties.³³ The optical response of the bimetallic systems are direct dependent on their chemical composition^{10,21,36}. For instance, in energy-dependent reflectance measurements one can clear see an

abrupt reduction of the spectra transitioning from the ultra-violet around 3.5 eV (Ag) to the visible around 2 eV (Au)²³. For pure Ag and Au, reflectance evaluated with DFT is found to have a slight blue shifted drop (Supplementary Fig. S1) due to the underestimation of the $d - sp$ interband transition obtained with the GGA-PBE functional, but still in good agreement with experimental responses³⁶. Overall, our results nicely agree with the ones found in the literature^{4,17,19–22,36,37}.

Complex Dielectric Function for Ag-Au Alloys

Figure 2 shows the imaginary part of the permittivity (ϵ_2) for the $\text{Ag}_{0.50}\text{Au}_{0.50}$ composition where an anisotropic behavior is observed in the calculated results (Figure 2 (a)). Conversely, the remaining structures are isotropic (see Supplementary Fig. S2). We evaluate ϵ_2 via the independent particle approximation (IPA) (see Methods for details). At the intraband transition region (energies < 3.5 eV) we see a split between the out-of-plane (y-direction) from the in-plane (xz-direction) component of ϵ_2 . To the best of our knowledge, for the aforesaid concentration, this is the first time that the anisotropic response is reported for the bulk configuration. The real part of the permittivity (ϵ_1), obtained from the Kramers-Kronig transformation of ϵ_2 ²³, also shows anisotropy (Supplementary Fig. S2(c)). Previously, Gong and co-authors performed the experimental analysis and the DFT calculations of the permittivity of Au-Ag alloys, where they showed a good agreement between the results. Also, they argued that the arrangement of the atoms in the $\text{Ag}_{0.50}\text{Au}_{0.50}$ structure lead to an anisotropic alloy, and emphasized that the optical transitions should occur only at symmetric Γ and R points of the Brillouin zone^{19,21}. Recently,

Figure 2. Imaginary part of the permittivity of the $\text{Ag}_{0.50}\text{Au}_{0.50}$ alloy. (a) Calculated in- (xz-direction) and out-of-plane (y-direction) components using the independent-particle approximation (IPA). (b) Experimental results obtained from the literature^{4,19–21}.

Cao Long and co-workers showed that the structure of the $\text{Ag}_{0.50}\text{Au}_{0.50}$ system is not cubic, but triclinic²². In both works, no evidence of an anisotropic optical response was reported. It is known that distinct methods of fabrication provide materials with different morphology and permittivity³⁸. When comparing reported values of ϵ_2 found in the literature we notice a larger discrepancy that reflects the same trend observed in our calculations (Fig. 2(b)).^{4, 19–21} Therefore, we attribute such difference as a result of the anisotropic optical response for the $\text{Ag}_{0.50}\text{Au}_{0.50}$ system. As shown in Fig. 2(a), the separation between the in- and out-of-plane components of the permittivity is in agreement with the literature results (Fig. 2(b)).

Origin of the anisotropy of the $\text{Ag}_{0.50}\text{Au}_{0.50}$ alloy

To elucidate the anisotropy of the $\text{Ag}_{0.50}\text{Au}_{0.50}$ alloy at the intraband transition region, we calculate the projected DOS (PDOS) over the d -orbitals of the valence band states (Supplementary Fig. S3). For the $\text{Ag}_{0.50}\text{Au}_{0.50}$ alloy, we notice that the d_{xz} orbital has a different PDOS from the d_{xy} and d_{yz} . Figure 3 shows the total PDOS projection (green lines), and the individual contribution of the Au atoms (purple-solid and dotted lines) and Ag atoms (red- dotted and solid lines). The d_{xy} , d_{xz} , and d_{yz} orbitals have the same shape but are aligned with the xy , yz , and xz planes, respectively (see inset of Fig. 3). Given the symmetry among them, we expect their contribution to the DOS to be symmetric. However, for the d_{xz} orbital we observe two peaks (Fig. 3(a)), at -2.25 eV, and -2.75 eV while for the d_{xy} and d_{yz} orbitals we see a single peak at -2.5 eV (green line on Figs. 3(b) and (c)). Also, there is an increase (decrease) in the intensity of the peak at -5.75 eV (-4.4 eV) (Supplementary Fig. S4(c)). Looking at the contribution of the individual atoms in the unit cell, the d_{xz} orbital presents an exchange in the contributions of the atoms for the least energetic peak with the main contribution coming from Au atoms instead of Ag. The next peak shows a more uniform contribution from both atoms, different from the Ag dominance seen in the other orbitals, with a broaden peak for Ag resulting in the decrease of the peak intensity. For the highest energetic peaks, the contribution of both atoms are found to be different in energy with the Au peak shifting towards the Fermi level. We see the same behavior in the pure Au and $\text{Ag}_{0.25}\text{Au}_{0.75}$ alloy (Supplementary Figs. S5(g)-(i) and Fig. S6). Finally, we observe a shoulder at -1.75 eV, absent in the others. Such peak may be related to the unbalance of charges in the xz -direction deforming the d_{xz} orbital. For the pure structures and the alloys with an unbalanced concentration between Ag and Au atoms, the

d_{xy} , d_{xz} , and d_{yz} orbitals contribute equally to the PDOS (Supplementary Figs. S4 and S5).

Figure 3. (a)-(c) Atoms-resolved contribution for the density of states projected over the d_{xy} , d_{xz} and d_{yz} orbitals for the $\text{Ag}_{0.50}\text{Au}_{0.50}$ alloys.

The charge density analysis agrees with the behavior of the PDOS. Figure 4(a)-(e) shows the charge distribution across the unit cells. Supplementary table S1 and Supplementary table S2 present the Bader³⁹ and Voronoi⁴⁰ partial charge analysis, respectively (See the Methods section for further details). Even though the charge analysis brings an overall behavior of the electronic occupation, there are regions of concentration of charge that resembles the spatial distribution of the orbitals. For both the Ag and Au, the charge is evenly distributed across the unit cell (Figs. 4(a) and (e), Supplementary table S1 and Supplementary table S2). The charge accumulated around the Au atoms is higher than that around the Ag ones agreeing with the different electronegativity of the Au and Ag³⁴. Supplementary table S1 shows charge distribution for the $\text{Ag}_{0.50}\text{Au}_{0.50}$, where we obtain 19.196 e and 18.803 e around the Au and Ag atoms, respectively. The total number of charge is 76 e , in accordance with the norm-conserving pseudo-potential employed in the calculations. Replacing an Au (Ag) atom with an Ag (Au) (Figs. 4(b) and (d)), the charge distribution slightly changes, with an nearly evenly distribution of the main charge over the unit cell (Supplementary table S1 and Supplementary table S2). However, for the $\text{Ag}_{0.50}\text{Au}_{0.50}$ alloy (Fig. 4(c)), we find the charge to change in the xz -direction due to the distribution of the atoms in the unit cell. Figures 4(f)-(o) show the integrated charge for the in-plane direction (Fig. 4(f)-(j)), and for the out-of-plane direction (Fig. 4(k)-(o)). The integrated charge of pure structures, as expected, is symmetric among planes. For the alloys, except for the $\text{Ag}_{0.50}\text{Au}_{0.50}$ one, the charge is, to a degree, symmetric between planes with the density highly resembling their pure counterparts. We understand this behavior

Figure 4. (a)-(e) Three-dimensional density of charge for the gold and silver structures and their alloys. (f)-(g) integrated two-dimensional density of charge in the xz -direction. (k)-(o) integrated two-dimensional density of charge in the y -direction.

in terms of the atom's contribution in the unit cells (Supplementary Fig. S5). For the Ag_{0.75}Au_{0.25} composition, two of Ag atoms have comparable contributions to the PDOS (Supplementary Figs. S5(d)-(f)). The remaining Ag atom has a contribution that resembles that of the Au atom, attributed to their equivalent structural positions within the unit cell. Therefore, the overall atomic contribution is somewhat symmetric among planes, directly reflecting in the charge density. For Ag_{0.25}Au_{0.75}, we observe a similar trend (Supplementary Figs. S5(g)-(i)). The in-plane density of charge of the Ag_{0.50}Au_{0.50} alloy (Fig. 4(h)) is clearly different from that of the out-of-plane (Fig. 4(m)), recovering the response of the d_{xy} , d_{xz} and d_{yz} orbitals contributions. The differences in the charge distribution should affect the electronic distribution, evidencing the polarity to the structure reported by Gong and co-workers²¹ for the Ag_{0.50}Au_{0.50}. Given the previous discussion, we believe that the anisotropy in the permittivity for the Ag_{0.50}Au_{0.50} structure is a direct consequence of the charge distribution in the electronic orbitals. The anisotropy occurs in the y -direction in detriment to the xz -direction response, in the same fashion as the d -orbitals.

Figure 5 shows the birefringence of the $\text{Ag}_{0.50}\text{Au}_{0.50}$ structure, where one can observe significant anisotropy for wavelengths above 600 nm. Here, we report the difference between the y- and the xz-direction of the refractive index (n) and the extinction coefficient (k). For comparison, n and k of all systems can be found on Supplementary Fig. S7. As expected, the pure structures and the remaining alloys show isotropic response. The structure with 50% Au and Ag could be employed as a birefringent material, broadening its range of applications as those in linear and non-linear anisotropic optics ^{26,28,29}.

Figure 5. Calculated birefringence for the refractive index and the extinction coefficient for the $\text{Ag}_{0.50}\text{Au}_{0.50}$ composition.

Conclusions

In summary, we used the density functional theory with the GGA exchange-correlation functional to determine the electronic structure, the density of states, and the optical response of gold-silver bimetallic structures in bulk form. For the pure gold and silver structures, as well as the alloys with 25% (75%) silver and 75% (25%) we obtained isotropic optical responses as expected for the cubic periodic unit cells. For the alloy with equal concentrations of gold and silver, namely $\text{Ag}_{0.50}\text{Au}_{0.50}$, the same was not valid. For such structure, we observed a difference between the y-direction and the xz-direction responses of the optical permittivity, mainly in the intraband energy regime. Since the dominant contribution to the intraband transitions comes from the d-orbitals in the valence band, we analyzed their projections on the density of states. We found that the d_{xz} orbital response were different from the d_{xy} and d_{yz} ones due to an unbalanced charge distribution in the structure. To the best of our knowledge, for the first time, we reported such anisotropic behaviour. Previous theoretical works obtained the permittivity of alloyed structures by

interpolating and fitting models using the pure samples as starting points. Consequently, no anisotropy could be found^{18,20,41}. Also, using first principle techniques, optical characterization of bimetallic structures were described as the a mean average of the three Cartesian directions^{4,19,21,22}. Likewise, this approach potentially hide any perspective of observing the anisotropic behavior shown. The present work shed light into the discrepancies present in the experimental and theoretical results found in the literature for Ag_{0.50}Au_{0.50} alloys. Moreover, one could obtain a birefringence by replacing Ag atoms with more massive elements, or with more pronounced relativistic effects and different electronegativities. The analysis of the non-linear optical properties could be performed, and we expected it to reveal anisotropic responses to the second-harmonic generation and third-order susceptibility²⁶.

Methods

Computational Details

Plane-waves-based DFT calculations were performed to obtain the optical and electronic properties of Ag-Au bimetallic structures, using the Quantum ESPRESSO package^{32,42,43}. We employed the Generalized-Gradient-Approximation (GGA) exchange-correlation functional with the Perdew–Burke–Ernzerhof (PBE) parametrization^{42,43}, and used the Hamann optimized scalar-relativistic norm-conserving pseudopotentials⁴⁴. The kinetic energy cutoff for the plane-wave basis expansion was 200 Ry.

Four-atom face-centered-cubic unitary cells were used as the initial structures, and their ground states were obtained by the total energy minimization method using the Broyden–Fletcher–Goldfarb–Shanno algorithm. All systems were relaxed until the energy and the forces on the atoms were lower than 10^{-5} Ry and 10^{-4} Ry/Å, respectively^{45,46}.

A uniform Monkhorst-Pack grid⁴⁷ with $16 \times 16 \times 16$ k-points in the Brillouin zone with no shift was chosen for the self-consistent-field calculation, where the threshold for the energy convergence was set as 10^{-12} Ry, kept the same throughout the simulations. For the band structures calculations we sampled a path between the high-symmetry points Γ -R-X- Γ -M-R.

For the electronic occupation, we adopted the Marzari-Vanderbilt cold smearing with a Gaussian spreading of 0.01 Ry on the Brillouin zone integration, taking into account the metallic occupation character of the systems⁴⁸. The density of states (DOS) calculations required a denser mesh of k-points.

Therefore, we used the non-self-consistent calculation with $32 \times 32 \times 32$ k-points with no shift, and an gaussian broadening of 0.1 Ry.

Permittivity

The wavelength-dependent permittivity ($\epsilon(\omega)$) was evaluated using the independent-particle approximation (IPA) through the *SIMPLE* code.²³ At the IPA level, the excitonic interaction is neglected. However, it is still suitable to obtain the optical properties of metallic systems through this method.^{33,36} The advantage of using the *SIMPLE* code relies on the use of optimal basis functions based on the Shirley integration approach, allowing for a very dense k-points sampling with affordable computational cost.^{36,49}

The interband transitions contribution to the optical permittivity for a negligible transferred momentum of the photons is given by²³

$$\epsilon_2^{inter}(\omega) = 1 - \frac{4\pi}{V} \sum_{\mathbf{k}, n \neq n'} \frac{|P_{\mathbf{k}, n \rightarrow n'}|^2}{(E_{\mathbf{k}n'} - E_{\mathbf{k}n})^2} \frac{f_{\mathbf{k}n} - f_{\mathbf{k}n'}}{\omega - (E_{\mathbf{k}n'} - E_{\mathbf{k}n}) + i\eta}, \quad (1)$$

where the summations are over the wave-vectors $\mathbf{k}$ in the first Brillouin zone, and over valence (n) and conduction (n') band states with energies $E_{\mathbf{k}n}$ and $E_{\mathbf{k}n'}$, respectively. $P_{\mathbf{k}, n \rightarrow n'}$ is the dipole matrix element denoting the transition between valence and conduction band states. The states occupation is given by the Fermi-Dirac distribution $f_{\mathbf{k}n(n')}$, and η is an empirical interband broadening to reproduce experimental scattering processes. The intraband transitions contribution to the optical permittivity is given by a Drude-like term dependent on the plasma frequency ω_d ,²³

$$\epsilon_2^{intra}(\omega) = -\frac{\omega_d^2}{\omega(\omega + i\gamma)}, \quad (2)$$

where γ is the empirical intraband broadening. To calculate the intraband and interband optical permittivity we employed a highly dense mesh with $72 \times 72 \times 72$ equally spaced k-points, with the threshold for the optimal basis set to 0.01bohr³. The intraband and interband broadenings were chosen to be 0.002 Ry and 0.013 Ry, respectively.

Partial charge analysis

Figure 4 shows isosurfaces of charge obtained from the DFT calculation and processed using the VESTA software.⁵⁰ The isolevel was set 0.1 for all the structures to allow for comparison. The integration in the charge density shown in Figs. 4 was also done using VESTA, with the results obtained with the projwfc.x software of Quantum ESPRESSO package³². We integrate the charge projection along the showed directions for a slice of the unit cell ranging from 20% to 40% of the cell's volume in that direction. We choose to include isosurfaces with the level between 2% to 7% of the total cell charge, where we spot the charge anisotropy among planes.

The charge distributed across the unit cell was also analysed via the Bader and Voronoi methods. The Bader analysis consists in separating the charge in regions using minimum density surfaces. The analysis was done employing the *Critic2*⁵¹ post-processing code that uses the Yu-Trinkle integration method³⁹. The results of the Bader partial charge analysis were presented in the Supplementary table 1. The Voronoi method is done directly by the Quantum ESPRESSO³² post-processing code together with the projected density of states. In such analysis, the charge distribution is given by portioning the cell space by the overlap in the charge density - called Voronoi cells⁴⁰.

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Author contributions statement

A.T.B. and M.R.S.D, conceived the project, H.M.L.C. performed the calculation(s). All authors analysed the results, wrote and reviewed the manuscript.

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Figure 1. Density functional theory (DFT) calculations of $\text{Ag}_x\text{Au}_{1-x}$ structures. (a)-(e) Schematics of the face centered cubic unitary cells. (f)-(j) Band structure calculations showing empty states ($>0\text{ eV}$) and the d-bands ($<0\text{ eV}$). (k)-(o) Calculated density of states (DOS) with total (black line) and projected-density of states (PDOS) for the s (red), p (green), and d-orbitals. The transition metal character of both Au and Ag structures is also observed in the alloys. This is characterized by the predominance of the d-orbital (light-gray line) contribution to the DOS.

Figure 2. Imaginary part of the permittivity of the $\text{Ag}_{0.50}\text{Au}_{0.50}$ alloy. (a) Calculated in- (xz -direction) and out-of-plane (y -direction) components using the independent-particle approximation (IPA). (b) Experimental results obtained from the literature^{4,19-21}.

Figure 3. (a)-(c) Atoms-resolved contribution for the density of states projected over the d_{xy} , d_{xz} and d_{yz} orbitals for the $\text{Ag}_{0.50}\text{Au}_{0.50}$ alloys.

Figure 4. (a)-(e) Three-dimensional density of charge for the gold and silver structures and their alloys. (f)-(g) integrated two-dimensional density of charge in the xz -direction. (k)-(o) integrated two-dimensional density of charge in the y -direction.

Figure 5. Calculated birefringence for the refractive index and the extinction coefficient for the $\text{Ag}_{0.50}\text{Au}_{0.50}$ composition.

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