Open Access Library Journal
2026, Volume 13, e14876
ISSN Online: 2333-9721
ISSN Print: 2333-9705

Localized Surface Plasmon Resonance, SERS, and Density of State Characterization of Phenols for Wastewater Remediation

—A DFT Approach

Michael Nakitare Waswa, Moses Wabwile Juma*, Samwel Muyiyi Mukhekhe

Department of Science, Technology, and Engineering, Kibabii University, Bungoma, Kenya
Email: *jmwabwire@gmail.com

How to cite this paper: Waswa, M.N., Juma, M.W. and Mukhekhe, S.M. (2026) Localized Surface Plasmon Resonance, SERS, and Density of State Characterization of Phenols for Wastewater Remediation. *Open Access Library Journal*, **13**: e14876.
https://doi.org/10.4236/oalib.1114876

Received: January 14, 2026
Accepted: March 15, 2026
Published: March 18, 2026

Abstract

Phenolic compounds pose a significant risk to the quality of water since they often remain persistent across the water supply chain. For the urban and peri-urban populations that leverage traditional water treatment approaches like boiling and filtration, phenols remain a key challenge since they are persistent micropollutants. In this work, the removal of these compounds has been demonstrated with the help of density functional theory, which, unlike experimental approaches, is less laborious and affordable. Localized surface plasmon resonance (LSPR), surface-enhanced Raman (SERS), and density of states were used to achieve label-free detection of the said molecule. The shifts in the plasmon band, as well as the Raman scatter bands, can be measured against different concentrations for trace detection of phenols and other contaminants. Raman scatter bands at 1120 cm^{-1}, 1192 cm^{-1}, 1345 cm^{-1}, and 1561 cm^{-1} emerged as key marker bands for spectral characterization of phenol molecules. Spectral shifts and intensity changes in such bands can be monitored for effective environmental remediation. Similarly, changes in band gap energy were monitored with the help of the density of state (DOS), and the charge distribution studies were carried out with the help of Mulliken analysis, demonstrating that there is a general reduction in the band gap after adsorption, with oxygen being the most electronegative element. Such changes in band gap and electronegativity studies can be used in the future for sensing of environmental contaminants.

Subject Areas

Computational Physics

Keywords

Phenols, Density of State, SERS, Density Functional Theory

1. Introduction

Access to clean water is a basic human right, but contamination from industrial waste, agricultural runoff, and natural pollutants presents serious risks to the natural ecosystems. Water treatment is vital because many areas, especially rural and suburban regions, lack centralized water infrastructure and depend on private wells or small systems that must be protected against pollutants, as stated by [1]. In rural setups, traditional water treatment methods include boiling, filtration, and solar disinfection, among others [2]. While the point-of-use methods are workable, especially for low-income households, they struggle with poor removal of chemical pollutants like heavy metals [3]. Consequently, such methods make it challenging to achieve water quality for the struggling populations [4], especially for persistent contaminants across the water supply chain.

Phenolic pollutants from agricultural activities pose a threat to water safety, especially for the rural population. These persistent micropollutants often find their way to drinking water sources, resulting in adverse health implications [5]. Using the context of Kenya's peri-urban set up, [6] noted that phenolic exotoxins are often present in raw river water, posing a significant threat to roadside food sold by vendors and hawkers who use nearby river water to prepare such food. The Kenya Water and Sanitation Regulatory Board (WASREB) reports that the acceptable safe quantities of Phenolic compounds in drinking and bottled water should be 0.002 Mg/L (Water Services Regulatory Board.gov). However, [6] reported that the level of phenolic compounds in sampled rivers and bottled water was way above the recommended limits. Higher phenolic compounds have also been reported in water bodies around grazing areas in the rural parts of South Africa, suggesting alternative treatment methods that guarantee water quality [7].

Conventional Raman and surface-enhanced Raman spectroscopy (SERS) have demonstrated notable utility in spectroscopy-based water treatment approaches. SERS technology works based on its single-molecule-level detection capability and the ability to achieve molecular fingerprint recognition. [8] Demonstrated the technology's synergistic effects of electrochemical and chemical enhancement, making the substrates reliable for single-molecule detection. [9] Achieved ultra-trace detection of pesticide residues, mycotoxins, and heavy metals, giving provision for on-site detection capabilities. Signal enhancement and spectral shifts have been used previously by [10] as key markers for environmental monitoring, including in water quality analysis. LSPR is often achieved with the use of nanomaterials.

Coupling nanotechnology and conventional Raman has emerged as a promising approach for enhancing water treatment processes, including the fabrication of water membranes for purification [11]. For instance, silver nanoparticles have previously been used in household water treatment systems as integrated filters and as effective antimicrobial agents that can kill bacteria, viruses, and fungi [12]. The nanoparticles are often leveraged due to their multifunctional properties, including excellent electrical conductivity, chemical stability, antibacterial effects, and optical characteristics [13]. These nanoparticles have been applied to water remediation as antibacterial agents, surface modifiers to increase adsorption capacities, sensors for detecting contaminants, and photocatalysts for degrading organic pollutants, as mentioned by [14]. The unique properties of silver nanoparticles can be tuned by controlling their size, morphology, and surface chemistry, making them highly effective in targeting water contaminants and microorganisms [15]. Besides, [11] note that silver nanoparticles are preferred in water treatment due to their unique optical, electrical, and magnetic properties that can be used in developing biosensor materials, composite fibers, and other electronic components.

Adsorption is widely used to remove contaminants from water systems since such processes are simple to design without harming byproducts [16]. Silver nanoparticles have specific characteristics, such as a high surface area and reactivity [17], surface plasmon resonance [18], surface-enhanced Raman scattering (SERS) [19] which are leveraged to remove phenolic compounds from water systems through adsorption. AgNPs have a small size that can exhibit a high surface area to volume ratio, which enhances their reactivity with phenolic compounds. Secondly, the nanoparticles show properties such as a strong surface plasmon resonance that varies from their bulk material, an adsorption property that can be used to monitor phenols and their derivatives. Lastly, the AgNPs help to amplify Raman signals of the adsorbed material, facilitating the detection and monitoring of phenols and their derivatives. Consequently, understanding these properties provides a clear roadmap for the adsorption of the nanomaterial in phenolic decontamination.

Density functional theory (DFT) has previously been used as an alternative approach to the laborious and costly laboratory procedures that have often been used to study surface area and reactivity, localized surface plasmon resonance (LSPR), and surface-enhanced Raman scattering (SERS) properties of AgNPs, applicable in adsorption studies. In studying silver nanoclusters on phenols, DFT offers a detailed understanding of molecular interactions and electronic properties at the atomic level, which are difficult to explore experimentally [10]. By calculating electronic density, molecular orbitals, energy states, and charge transfer mechanisms, DFT helps clarify how silver clusters interact with phenolic compounds and how these interactions affect optoelectronic properties relevant for photocatalytic degradation and adsorption [20]. These insights guide the development of more effective silver-based nanomaterials for sustainable wastewater treatment. Consequently, this work will leverage DFT as a less costly and time-conscious technique that helps to study the LSPR, SERS, and surface area and reactivity property of AgNPs, applicable in the adsorption of phenolic compounds towards water treatment applications.

2. Computational Details

The atomic structures of silver nano clusters were imported as a .csv file from the

Quantum Cluster Database. These structures were visualized using Gauss View software. The Gaussian 09W program package was used for DFT calculations at the Becke's three-parameter functional and Lee-Yang-Parr hybrid functional (B3LYP) level of theory. The LANL2DZ basis set was applied for silver atoms, with the 6-31G++ (d, p) basis set for other atoms. Calculations were performed for ground state geometry optimization in air. To obtain the electron density distribution, molecular orbitals, and energy eigenvalues, a B3LYP hybrid functional was employed. Raman frequencies were calculated on the optimized structure using the same basis set and level of theory, with the Gaussian 09 program. To determine energy, oscillator strength, and wavelength, TD-DFT calculations were conducted. Charge transfer analysis involved examining molecular orbitals and electron density difference maps using Natural Bond Orbital (NBO) or Mulliken population analysis to quantify electron transfer and interaction strength. PDOS was used to analyze contributions from Ag and phenol molecules.

3. Results and Discussions

3.1. Geometry Optimization

Ag18, phenols, and Ag18-phenol complex moieties were optimized in air at the B3LYP level of theory using Gaussian 09 software. Ag-18 was preferred in this work due to its molecule-like properties. Previously, [21] reported that Ag-18 is preferred due to its unique bonding properties within the metal core. The specific and atomic level structure of the Ag-18 also provides a significantly higher antimicrobial efficiency and better stability as compared to other nanoclusters and conventional silver nanoparticles. Using mass spectrometry, [22] demonstrated that Ag-18's atom-precise design (<2 nm) yields superior geometric rigidity, with minimal core fragmentation. **Figure 1** shows the optimized structure of the Ag-18 nanocluster and that of phenols. As indicated in **Figure 1**, phenols have a single hydroxyl group with an oxygen atom that is electronegative and which will play a key role in the adsorption process.

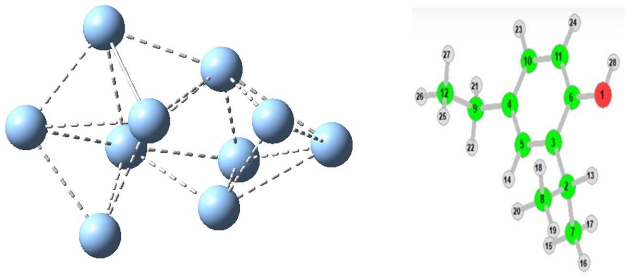

Figure 1. Optimized structure of Ag-18 nanocluster (left) and phenols (right).

As shown in **Figure 1**, Phenols have a hydroxyl (OH) group that is directly attached to the benzene ring, replacing one of the hydrogen atoms. In this work, the 3D molecule was directly imported from PubChem before being optimized using Gaussian 09.

3.2. Raman and SERS Spectra of Phenols

Raman and SERS spectral characterization of phenols was carried out to ascertain the possible changes in band position after phenols are adsorbed on silver nanoparticles. In the Gauss View window, phenols were allowed to embed on the metallic nanoclusters with the oxygen atom of phenols being the target atom in the attachment, as shown in **Figure 2**. Oxygen has previously been reported by [23] to be the most electronegative and, as such, would help to form a stronger bond during adsorption.

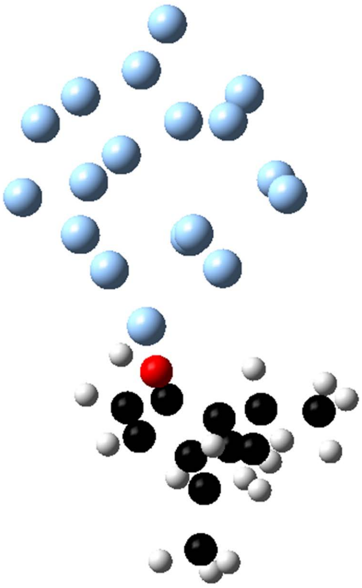

Figure 2. Silver nanoclusters embedded on phenolic compound in Gauss view.

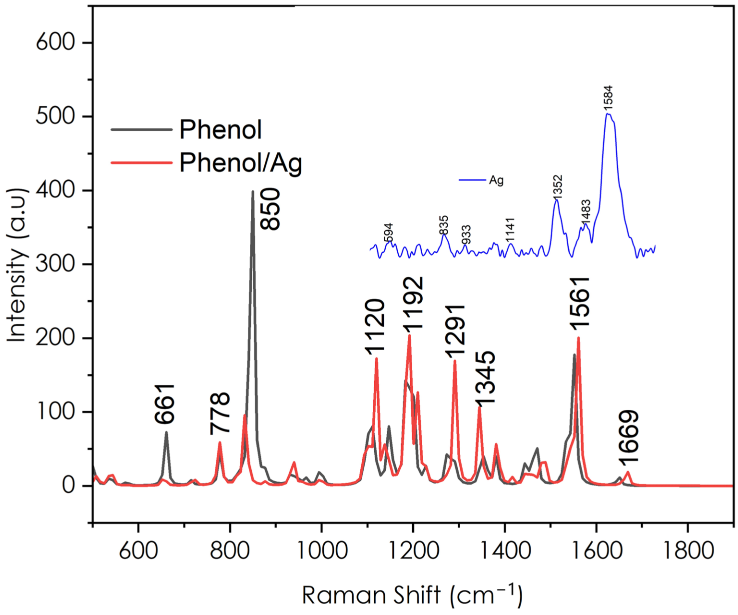

Figure 3. Simulated Raman and SERS spectra of phenols (inset: spectra of silver NPs).

The results depicted in **Figure 3** show that phenols exhibit very strong Raman bands within the active spectral window between 600 cm^{-1} and 1700 cm^{-1} due to the symmetric stretching mode of the aromatic ring (C = C). Some of the bands between 1100 cm^{-1} and 1300 cm^{-1} tend to be isoenergetic, with almost identical spectral features. The simulated spectra of phenols were found to be similar to those reported by other authors for both simulated and experimental data. For instance, [24] noted that two ring deformation modes around 1500 - 1600 cm^{-1} offer a potential route in gaining information about phenolic compounds in the macroenvironment. Density functional theory predictions given by [25] also showed that phenols have predominant Raman scatter bands at 850 cm^{-1}, 1120 cm^{-1}, 1291 cm^{-1}, and 1560 cm^{-1} assigned to C = C and C = O symmetric vibrational bonds using vibrational energy distribution (VEDA).

Adsorbing phenols on silver nanoparticles had notable implications on the phenols' Raman bands. As noted in **Figure 2**, some of the bands reported higher signal intensity after adsorbing the molecule on silver nanoparticles. The peaks at 1120 cm^{-1}, 1291 cm^{-1}, and 1345 cm^{-1} reported an almost similar threefold enhancement factor. [26] Defines the enhancement factor as the key parameter for the assessment of the substrate performance. In this case, the signal enhancement factor was given as the ratio of the enhanced signal to the non-enhanced signal for a specific Raman scatter band. The enhancement factor directly quantifies the ability of silver nanoparticles as a substrate that can amplify phenol molecule signals for trace-level contaminant detection [27].

The other observation made from **Figure 2** is the shift in some of the Raman scatter bands. The bands that reported a red shift after phenols are adsorbed on the silver nanoparticles include 1120 cm^{-1}, 1291 cm^{-1}, 1561 cm^{-1}, and 1669 cm^{-1}. All these shifts were characteristic of the C = C and C = O stretching vibrations, while 1345 cm^{-1} (C-O breathing vibrational mode) had a slight blue shift after adsorption. Because these modes are structurally specific, even slight band position changes can indicate that phenols are present and interacting with their microenvironment in water [28]. [29] Also argues that tracking these shifts as a function of time or concentration enables early detection and even speciation of phenolic contaminants.

3.3. Localized Surface Plasmon Resonance

Silver nanoparticles were used both as substrates (in SERS) for signal enhancement and spectral shifts characterization, and as nanostructures for localized surface plasmon resonance sensing of phenols. The plasmon band of silver nanoparticles presents a strong optical effect for collective oscillations, such that by monitoring the LSPR peak shift (change in wavelength) caused by the binding material, it is possible to achieve a label-free detection of the analyte. In this work, the high refractive index sensitivity of silver nanoparticles was monitored by adsorbing phenols on silver nanoparticles and then measuring the change in the LSPR position using simulated absorbance spectra, as shown in **Figure 4**.

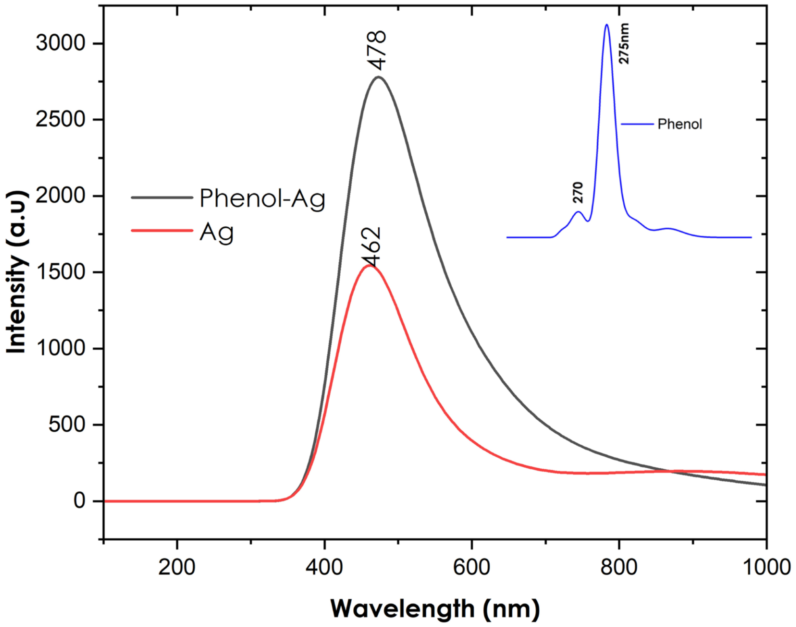

Figure 4. UV-VIS spectra of Silver Nanocluster (Ag18) and phenols/AgNCs complex. Inset is the absorbance spectra of phenols.

As shown in **Figure 4**, phenols have two absorbance bands at 270 nm and 275 nm. The simulated band was similar to what has been reported by other scholars, such as [30]-[32]. Therefore, the UV-VIS calculations implemented using DFT reproduced the experimental results by almost 100% as reported by other scholars. Secondly, the absorbance band of silver nanoclusters was 462 nm, which is almost similar to what was reported by other scholars. [33] Reported the plasmon band at 450 nm using an experimental procedure, while [34] used DFT and estimated the absorbance band of silver nanoparticles to be 426 nm. The deviations in the absorbance values reported for this work could be attributed to the differences in the number of atoms used in the nanoclusters.

As noted in **Figure 4**, there is a slight redshift in the localized surface plasmon resonance band of the silver nanocluster from 462 nm to 478 nm. The +16 nm change is significant in environmental monitoring applications, as explained by [35]. According to [36], silver nanoparticles are more sensitive to changes in both the local and bulk environment. Introducing phenols to silver nanoclusters changes the refractive index of the local environment, a move that allows label-free trace and ultra-trace detection of phenols and other contaminants in the environment. The results reported in **Figure 4** show that silver nanoparticles are very sensitive to any changes in the optical properties of the surrounding medium, like the adsorption of the target analyte (phenols) on the nanomaterials. Therefore, the silver nanoparticles are important candidates for monitoring phenols within the environment.

3.4. Density of State

In this part, Density functional theory was employed as a synergistic approach that provides a molecular-level understanding of the electrical and optical properties of silver nanoclusters when adsorbed with phenols. The focus was on understanding the adsorption sites and the electron transfer, both of which are key in elucidating the adsorption process of phenol removal from water. [37] Leveraged the density of state, which reflects the density of kinetic energy, to ascertain the confinement and scattering of charge. Density of states (DOS) was used to describe how many quantum states are available at each energy in a system, and it is a central bridge between electronic structure, spectroscopy, and adsorption phenomena. DOS was evaluated before (**Figure 5**) and after adsorption (**Figure 6**) to ascertain changes in the band gap energy, which is also an important parameter in biosensing applications.

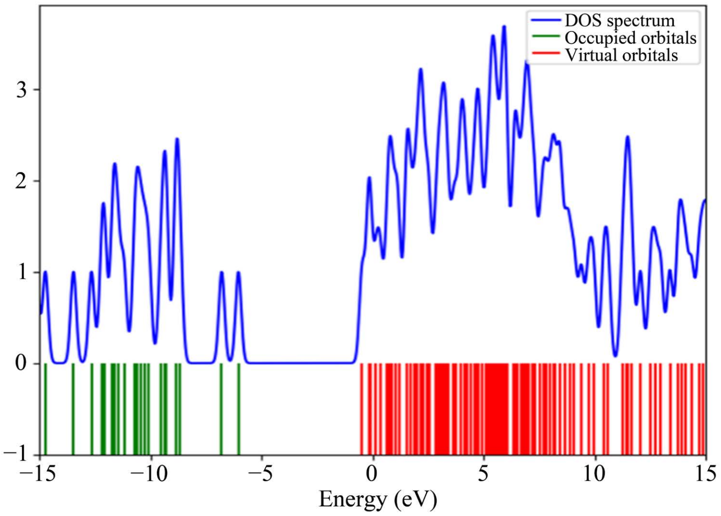

Figure 5. Density of state spectra of phenols.

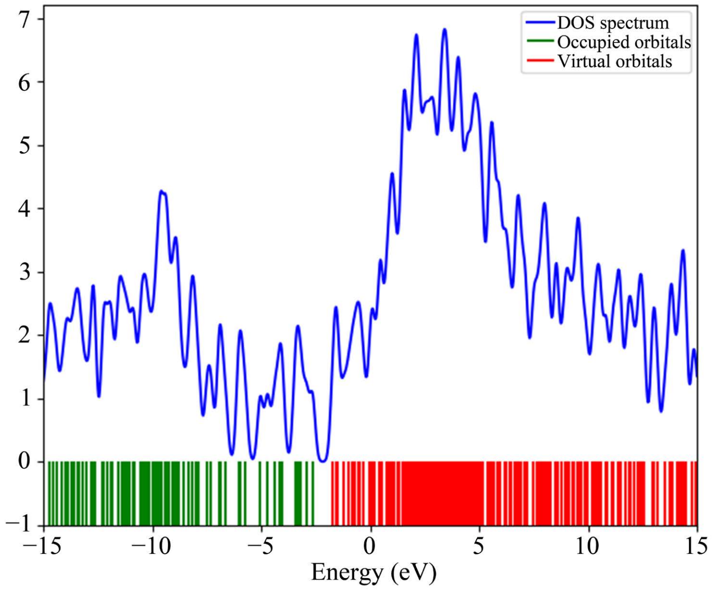

Figure 6. Density of state spectra of phenols adsorbed on AgNPs.

As shown in **Figure 6**, there is a general reduction in the band gap energy after phenols are adsorbed on silver nanoparticles. The band gap reduced from approximately 7 eV to less than 2 eV. [38] Asserts that a reduction in the band gap after adsorption enhances a material's light absorption range and charge-carrier generation, enabling more sensitive optical detection of environmental analytes, such as water pollutants, through spectroscopic changes. In sensing applications, the narrowing of the band gap also translates to improved sensor sensitivity by amplifying optical responses to low analyte levels, as even trace adsorption triggers detectable spectral changes. The observations in this case are critical to developing a label-free analytical technique for monitoring environmental pollutants.

3.5. Mulliken Charge Distribution

Table 1. Mulliken charges for selected elements for phenol molecules adsorbed on Ag18.

Atoms	Atomic charges (Mulliken) using B3LYP/6-311++G (d, p)
C1	0.187
C2	0.161
C3	0.159
C4	0.158
C5	0.168
C6	0.179
C7	0.157
C8	0.148
C9	0.166
Ag1	0.184
Ag2	0.182
Ag3	0.165
Ag4	0.158
Ag5	0.108
Ag6	−0.215
Ag7	−0.201
Ag8	−0.177
Ag9	−0.021
O	−0.628
H1	0.147
H2	0.148
H3	0.138
H4	0.175
H5	0.179
H6	0.165
H7	0.197

The interaction between silver and phenols was also explained with the help of atomic charge analysis. [39] Notes that the Mulliken charge is directly related to the vibrational properties of the molecule and also quantifies how the electronic structure charges under atomic displacement. Therefore, using the charge distribution, it is possible to underscore the chemical bonds present in the molecule. **Table 1** shows the Mulliken charges of some of the carbon, hydrogen, and oxygen atoms for phenols and those of silver atoms during the adsorption process at a specific level of theory.

All the Carbon and hydrogen atoms in the molecule have positive charges, while some silver atoms and oxygen show negative charges, with oxygen being the most electronegative. **Figure 7** shows a summary of the charge distribution.

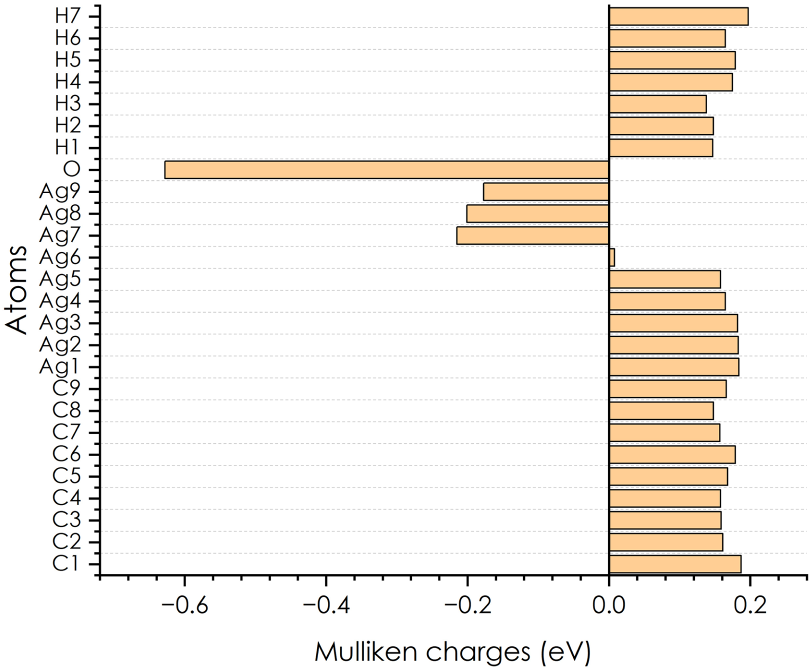

Figure 7. Mulliken charge distribution for Phenols adsorbed on silver nanocluster.

The Mulliken charge distribution shows that oxygen is the most electronegative atom, giving it the highest tendency to attract and bond to the electropositive silver during the adsorption process. Therefore, functional groups with an oxygen molecule will play an important role in defining the interaction between silver and oxygen during the adsorption process.

4. Conclusion

In this work, density functional theory was employed as a feasible approach to the rather expensive and time-consuming experimental procedures for label-free detection of phenol contaminants. The DFT approach helped to ascertain the optical properties, such as localized surface plasmon resonance and surface-enhanced Raman scattering behavior of silver nanoparticles in trace detecting phenols within the environment. The optical properties were computationally determined based on the localized surface plasmon band, Raman frequencies, and the changes in band gap energies. The Mulliken charge analysis also showed that oxygen is the most electronegative element that would significantly participate in the adsorption process through relevant functional groups. The results showed that it is possible to leverage the capability of DFT to demonstrate the place of silver nanoparticles and nanotechnology in general for environmental monitoring of pollutants.

Conflicts of Interest

The authors declare no conflicts of interest.

References

[1] Peter-Varbanets, M., Zurbrügg, C., Swartz, C. and Pronk, W. (2009) Decentralized Systems for Potable Water and the Potential of Membrane Technology. *Water Research*, **43**, 245-265. https://doi.org/10.1016/j.watres.2008.10.030

[2] Sobsey, M.D., Stauber, C.E., Casanova, L.M., Brown, J.M. and Elliott, M.A. (2008) Point of Use Household Drinking Water Filtration: A Practical, Effective Solution for Providing Sustained Access to Safe Drinking Water in the Developing World. *Environmental Science & Technology*, **42**, 4261-4267. https://doi.org/10.1021/es702746n

[3] Geremew, A. and Damtew, Y.T. (2019) Household Water Treatment Using Adequate Methods in Sub-Saharan Countries: Evidence from 2013–2016 Demographic and Health Surveys. *Journal of Water*, *Sanitation and Hygiene for Development*, **10**, 66-75. https://doi.org/10.2166/washdev.2019.107

[4] de Andrade Costa, D., Soares de Azevedo, J.P., dos Santos, M.A. and dos Santos Facchetti Vinhaes Assump, R. (2020) Water Quality Assessment Based on Multivariate Statistics and Water Quality Index of a Strategic River in the Brazilian Atlantic Forest. *Scientific Reports*, **10**, Article No. 22038. https://doi.org/10.1038/s41598-020-78563-0

[5] Mhlongo, N.L., Akharame, M.O., Pereao, O., Human, I.S. and Opeolu, B.O. (2024) Phenolic Compounds Occurrence and Human Health Risk Assessment in Potable and Treated Waters in Western Cape, South Africa. *Frontiers in Toxicology*, **5**, Article 1269601. https://doi.org/10.3389/ftox.2023.1269601

[6] Muitta, E. (2024) Phenolic Ecotoxins in River Water: Survey on Knowledge and Practices of Road-Side Food Vendors Operating along River Chania Bank Fringes in Thika Sub-County, Kenya. *Natural Science Journal*, **5**, 33-47. https://doi.org/10.47941/nsj.2316

[7] Rapiya, M., Slayi, M. and Truter, W. (2025) A Review of Phenolic Compounds in Water Bodies of Grazing Areas. *Discover Water*, **5**, Article No. 69. https://doi.org/10.1007/s43832-025-00280-4

[8] Ong, T.T.X., Blanch, E.W. and Jones, O.A.H. (2020) Surface Enhanced Raman Spectroscopy in Environmental Analysis, Monitoring and Assessment. *Science of the Total Environment*, **720**, Article 137601. https://doi.org/10.1016/j.scitotenv.2020.137601

[9] Xue, R.S., Dai, J.Y., Wang, X.J., *et al.* (2025) Research Progress of Surface-Enhanced Raman Scattering (SERS) Technology in Food, Biomedical, and Environmental Monitoring. *Photonics*, **12**, Article 809.

[10] Chen, Y. and Ming, H. (2012) Review of Surface Plasmon Resonance and Localized

Surface Plasmon Resonance Sensor. *Photonic Sensors*, **2**, 37-49. https://doi.org/10.1007/s13320-011-0051-2

[11] Spoiala, A., Ficai, D., Gunduz, O., Ficai, A. and Andronescu, E. (2018) Silver Nanoparticles Used for Water Purification. *Advanced Materials and Technologies for Environmental Applications*, **2**, 15. https://www.researchgate.net/publication/360562980_SILVER_NANOPARTICLES_USED_FOR_WATER_PURIFICATION

[12] Bhardwaj, A.K., Sundaram, S., Yadav, K.K. and Srivastav, A.L. (2021) An Overview of Silver Nano-Particles as Promising Materials for Water Disinfection. *Environmental Technology & Innovation*, **23**, Article 101721. https://doi.org/10.1016/j.eti.2021.101721

[13] Zahoor, M., Nazir, N., Iftikhar, M., Naz, S., Zekker, I., Burlakovs, J., *et al.* (2021) A Review on Silver Nanoparticles: Classification, Various Methods of Synthesis, and Their Potential Roles in Biomedical Applications and Water Treatment. *Water*, **13**, Article 2216. https://doi.org/10.3390/w13162216

[14] Tripathy, J., Mishra, A., Pandey, M., Thakur, R.R., Chand, S., Rout, P.R., *et al.* (2024) Advances in Nanoparticles and Nanocomposites for Water and Wastewater Treatment: A Review. *Water*, **16**, Article 1481. https://doi.org/10.3390/w16111481

[15] Sahu, M., Ganguly, M. and Sharma, P. (2024) Role of Silver Nanoparticles and Silver Nanoclusters for the Detection and Removal of Hg(II). *RSC Advances*, **14**, 22374-22392. https://doi.org/10.1039/d4ra04182h

[16] Ramírez-Hernández, M., Cox, J., Thomas, B. and Asefa, T. (2023) Nanomaterials for Removal of Phenolic Derivatives from Water Systems: Progress and Future Outlooks. *Molecules*, **28**, Article 6568. https://doi.org/10.3390/molecules28186568

[17] Syafiuddin, A., Salmiati, S., Jonbi, J. and Fulazzaky, M.A. (2018) Application of the Kinetic and Isotherm Models for Better Understanding of the Behaviors of Silver Nanoparticles Adsorption onto Different Adsorbents. *Journal of Environmental Management*, **218**, 59-70. https://doi.org/10.1016/j.jenvman.2018.03.066

[18] Deng, S., Wang, P. and Yu, X. (2017) Phase-Sensitive Surface Plasmon Resonance Sensors: Recent Progress and Future Prospects. *Sensors*, **17**, Article 2819. https://doi.org/10.3390/s17122819

[19] Lana-Villarreal, T., Pérez, J.M. and Gómez, R. (2004) Surface Enhanced Raman Spectroscopy for Adsorption Studies on Semiconductor Nanostructured Films. *Surface Science*, **572**, 329-336. https://doi.org/10.1016/j.susc.2004.09.009

[20] Malekzad, H., Sahandi Zangabad, P., Mohammadi, H., Sadroddini, M., Jafari, Z., Mahlooji, N., *et al.* (2018) Noble Metal Nanostructures in Optical Biosensors: Basics, and Their Introduction to Anti-Doping Detection. *TrAC Trends in Analytical Chemistry*, **100**, 116-135. https://doi.org/10.1016/j.trac.2017.12.006

[21] Chen, Z., Walsh, A.G., Wei, X., Zhu, M. and Zhang, P. (2022) New Insights into the Bonding Properties of [Ag25(SR)18]-Nanoclusters from X-Ray Absorption Spectroscopy. *The Journal of Physical Chemistry C*, **126**, 12721-12727. https://doi.org/10.1021/acs.jpcc.2c04482

[22] Guha, R., Malola, S., Rafik, M., Khatun, M., Gonzàlez-Rosell, A., Häkkinen, H., *et al.* (2024) Fragmentation Patterns of DNA-Stabilized Silver Nanoclusters under Mass Spectrometry. *Nanoscale*, **16**, 20596-20607. https://doi.org/10.1039/d4nr03533j

[23] Juma, M.W., Birech, Z., Mwenze, N.M., Ondieki, A.M., Maaza, M. and Mokhotjwa, S.D. (2024) Localized Surface Plasmon Resonance Sensing of Trenbolone Acetate Dopant Using Silver Nanoparticles. *Scientific Reports*, **14**, Article No. 5721. https://doi.org/10.1038/s41598-024-56456-w

[24] Larsen, K.L. and Barsberg, S. (2010) Theoretical and Raman Spectroscopic Studies of Phenolic Lignin Model Monomers. *The Journal of Physical Chemistry B*, **114**, 8009-8021. https://doi.org/10.1021/jp1028239

[25] Billes, F. and Mohammed‐Ziegler, I. (2007) Vibrational Spectroscopy of Phenols and Phenolic Polymers. Theory, Experiment, and Applications. *Applied Spectroscopy Reviews*, **42**, 369-441. https://doi.org/10.1080/00102200701421748

[26] Cara, E., Mandrile, L., Sacco, A., Giovannozzi, A.M., Rossi, A.M., Celegato, F., *et al.* (2020) Towards a Traceable Enhancement Factor in Surface-Enhanced Raman Spectroscopy. *Journal of Materials Chemistry C*, **8**, 16513-16519. https://doi.org/10.1039/d0tc04364h

[27] Jayawardhana, S., Mazzolini, A.P., Stoddart, P.R., Champion, P.M. and Ziegler, L.D. (2010) Trace Level Detection of Water Contamination by Sers. *AIP Conference Proceedings*, **1267**, 1063-1064. https://doi.org/10.1063/1.3482296

[28] Marley, N.A., Mann, C.K. and Vickers, T.J. (1984) Determination of Phenols in Water Using Raman Spectroscopy. *Applied Spectroscopy*, **38**, 540-543. https://doi.org/10.1366/0003702844555304

[29] Stehle, S. and Braeuer, A.S. (2019) Hydrogen Bond Networks in Binary Mixtures of Water and Organic Solvents. *The Journal of Physical Chemistry B*, **123**, 4425-4433. https://doi.org/10.1021/acs.jpcb.9b02829

[30] Murillo-Acevedo, Y.S., Giraldo, L., Poon, P.S., Matos, J. and Moreno-Piraján, J.C. (2021) The Cramer's Rule for the Parametrization of Phenol and Its Hydroxylated Byproducts: UV Spectroscopy vs. High Performance Liquid Chromatography. *Environmental Science and Pollution Research*, **28**, 6746-6757. https://doi.org/10.1007/s11356-020-10897-8

[31] Boulet, J.C., Ducasse, M.A. and Cheynier, V. (2017) Ultraviolet Spectroscopy Study of Phenolic Substances and Other Major Compounds in Red Wines: Relationship between Astringency and the Concentration of Phenolic Substances. *Australian Journal of Grape and Wine Research*, **23**, 193-199. https://doi.org/10.1111/ajgw.12265

[32] Garncarzová, M., Veselý, L., Kim, B., Kim, K. and Heger, D. (2025) Spectroscopic Characterization of Phenol in Frozen Aqueous Solution and on the Ice Surface. *Spectrochimica Acta Part A*: *Molecular and Biomolecular Spectroscopy*, **335**, Article 125948. https://doi.org/10.1016/j.saa.2025.125948

[33] Han, F., Li, J., Wang, W., Wang, M. and Li, L. (2022) Synthesis of Silver Nanoclusters by Irradiation Reduction and Detection of Cr^{3+} Ions. *RSC Advances*, **12**, 33207-33214. https://doi.org/10.1039/d2ra06536c

[34] Rabilloud, F. (2013) UV-Visible Absorption Spectra of Metallic Clusters from TDDFT Calculations. *The European Physical Journal D*, **67**, Article No. 18. https://doi.org/10.1140/epjd/e2012-30448-x

[35] Murray, W.A., Auguié, B. and Barnes, W.L. (2009) Sensitivity of Localized Surface Plasmon Resonances to Bulk and Local Changes in the Optical Environment. *The Journal of Physical Chemistry C*, **113**, 5120-5125. https://doi.org/10.1021/jp810322q

[36] Mahmoudpour, M., Ezzati Nazhad Dolatabadi, J., Torbati, M. and Homayouni-Rad, A. (2019) Nanomaterials Based Surface Plasmon Resonance Signal Enhancement for Detection of Environmental Pollutions. *Biosensors and Bioelectronics*, **127**, 72-84. https://doi.org/10.1016/j.bios.2018.12.023

[37] Iqrar, U., Masood, U., Alarfaji, S.S., Iqbal, T., Majid, A. and Isa Khan, M. (2024) Adsorption Behavior of Different Cresols on Bismuthene: A DFT Study. *RSC Advances*, **14**, 18787-18797. https://doi.org/10.1039/d4ra02933j

[38] Quhe, R., Fei, R., Liu, Q., Zheng, J., Li, H., Xu, C., *et al.* (2012) Tunable and Sizable Band Gap in Silicene by Surface Adsorption. *Scientific Reports*, **2**, Article No. 853. https://doi.org/10.1038/srep00853

[39] Ramalingam, S., Karabacak, M., Periandy, S., Puviarasan, N. and Tanuja, D. (2012) Spectroscopic (Infrared, Raman, UV and NMR) Analysis, Gaussian Hybrid Computational Investigation (MEP Maps/HOMO and LUMO) on Cyclohexanone Oxime. *Spectrochimica Acta Part A*: *Molecular and Biomolecular Spectroscopy*, **96**, 207-220. https://doi.org/10.1016/j.saa.2012.03.090