IOCAT 2026 Conference

The 1st International Online Conference on Atoms

29–30 January 2026 | Online

MDPI

DFT studies on 2-(3-methylureido)acetic acid (MUA)-functionalized Ag_6 metallic nanocluster

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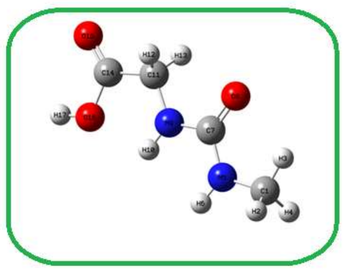
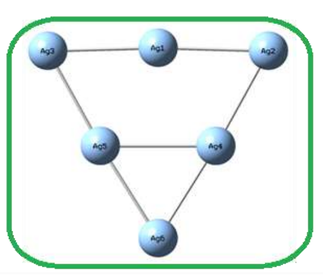
INTRODUCTION & AIM

Metallic nanoclusters can be synthesized in a wide range of sizes and stoichiometries by incorporating coinage metals. Among the different sizes of nanoclusters, six atom clusters are of particular interest, as they represent the smallest experimentally realized species in both homo- and bimetallic forms, with or without passivating ligands. 2-(3-Methylureido)acetic acid is selected in this study due to its distinctive charge transfer characteristics.

This study uses DFT to examine the interaction between an Ag_6 nanocluster and 2-(3-methylureido)acetic acid (MUA). Different binding configurations are analyzed to identify the most stable adsorption site and assess the electronic properties of the MUA–Ag_6 system for potential nanoscale applications.

METHOD





All DFT computations were carried out with the Gaussian 16 package, employing B3LYP/ LANL2DZ. For the Ag_6 system, three possible configurations were used: metal cluster near to C=O as D1; near to COOH as D2; and near to NH as D3. Geometry optimizations were validated through harmonic vibrational frequency analyses, confirming the absence of imaginary modes.

RESULTS & DISCUSSION

For the MUA (Figure 1a) the most reactive sites (Figure 1c) are O atoms (reddish yellow) and H atoms (bluish). The HOMO is over the entire drug except C=O and COH while LUMO is over the COOH and nearby CH_2 (Figure 1b).

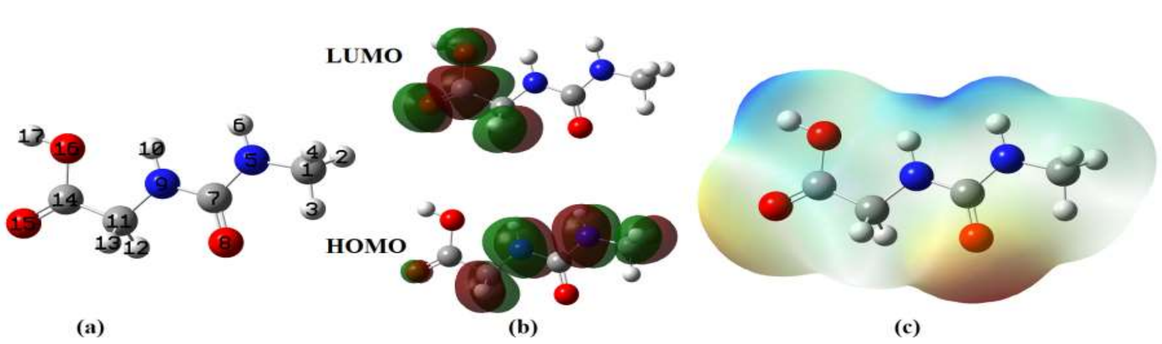


Figure 1. MUA's (a) optimized geometry (b) FMOs (c) MEP plots

The dipole moments (DM) are varying in the order D1 (10.85) > D2 (10.30) >D3 (4.83) while that of MUA is 5.40 Debye and for D3 configuration, DM is less than that of MUA. The polarizability values of the complexes are very much greater than that of MUA. The interaction between Ag_6 cluster and drug is given by the separation distance of Ag to O8 as 2.3619 for D1; Ag to O15 separation of 2.4482 for D2 and Ag to N9 separation of 2.5539 Å for D3..

Table 2: Calculated energy , dipole moment and polarizability

System	E(B3LYP) (Hartree)	Dipole Moment (Debye)	Polarizability (a.u.)
MUA	-492.3797	5.3974	63.8680
Ag6	-874.8166	0.0000	283.2633
D1 complex	-1367.2138	10.8530	362.1757
D2 complex	-1367.2070	10.2985	361.2500
D3 complex	-1367.2037	4.8266	360.9913

Table 1: Calculated Adsorptiion Energy

Configuration	Adsorption Energy (kcal mol^{-1})
D1	-11.04
D2	-6.73
D3	-4.79

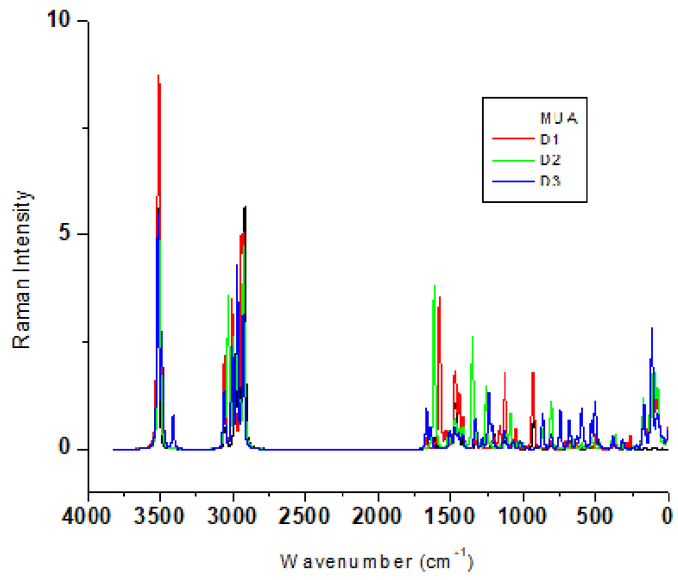


Figure 2. Theoretical Raman Spectra

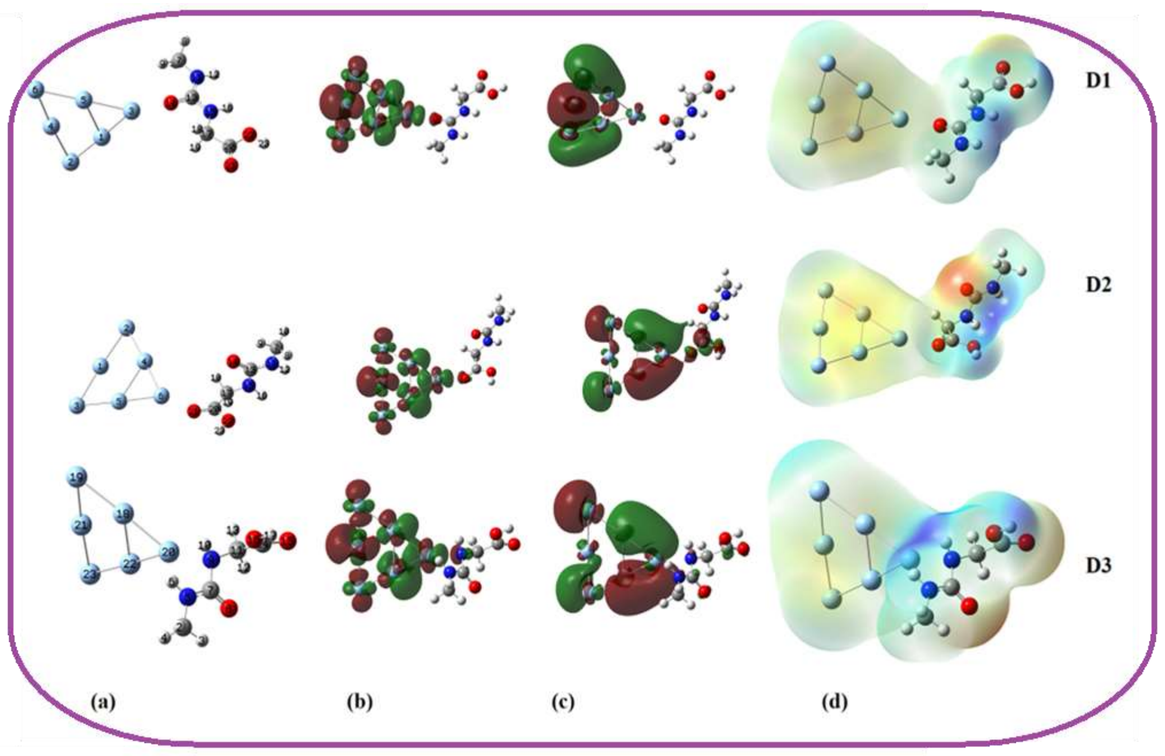


Figure 3. (a) MUA-Ag6 (b) HOMO (c) LUMO (d) MEP plots

CONCLUSION

The interaction of MUA with the Ag_6 nanocluster has been analyzed using DFT calculations. Among the studied configurations, D1 shows the strongest adsorption and highest stability. Enhanced Raman response, dipole moment and polarizability upon complex formation indicate notable charge transfer, highlighting the potential of the MUA–Ag_6 system for nanoscale electronic and sensing applications.

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Acknowledgment:

I would like to express my sincere gratitude to Jamelah S. Al-Otaibi *. Department of Chemistry, College of Science, Princess Nourah Bint Abdulrahman University, P.O. Box 84428, Riyadh, 11671, Saudi Arabia for her assistance with Gaussian-based computational calculations used in this study.*