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## Electronic properties and the electron distribution of graphamid doped: A DFT study

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### Abstract

Recently, a method for creating a novel monomer known as 2,4,6- tris((diphenylmethylene) amino) benzene-1,3,5-tricarbaldehyde) was disclosed. This monomer is anticipated to find use in many electronic devices and applications. In this perspective, the graphamid structure with and without doping, obtaining enhanced electronic properties. Atoms of transition elements, including Sc, Ti, Fe, Ni, Cu, and Nb, were added to the pure complex. Based on the B3LYP function and the basis set 6-31G(d), the density functional theory (DFT) method was used for the geometric optimization and computations for all compounds. The electronic characteristics of pure graphamid, including its energy gap, electrophilicity, hardness, softness, and electronegativity, are considerably changed when different metals are added. These modifications affect the doped structures' potential ultizes, stability, and reactivity. Through comprehension of these characteristics, the material can be tailored for particular uses in sensor technology, optoelectronics, and catalysis. These results are further supported by the molecular structure visualization and the infrared spectrum, which show variations in vibrational modes and electronic density. The energy gap values of the compounds before and after doping are in the semiconductor region and have a range of values (1.084046-1.512876 eV) that give freedom in choosing the compound that suits the application and the desired device. It was found that the best two compounds that can be recommended in the design of sensors are graphamid with copper and graphamid with scandium, and this is attributed to their high reactivity. While graphamid compounds doped with iron or titanium have high stability and low reactivity, they can be recommended for working as catalysts or as a delivery for treatment.

**Keywords:** Energy gap, graphamid, electronic properties, DFT, transition element

### 1. Introduction

A new area of material science called nanomaterials <sup>[1]</sup> has the potential to completely transform a number of different sectors. They have special qualities because of their nanoscale size, which leads to new developments in energy, electronics, medicine, and other fields. Unlocking the full potential of research and technology will depend on addressing the obstacles that come with using them as they improve <sup>[1-4]</sup>. The synthesis of a novel monomer <sup>[5]</sup>, 2,4,6-tris((diphenylmethylene)amino)benzene-1,3,5-tricarbaldehyde) <sup>[6, 7]</sup>, also referred to as "graphamid", a new high-performance material, is described in a recent technical report <sup>[5, 8]</sup>. It is composed of a single benzene ring with three pendant aldehyde groups that alternate with three benzophenone imine groups. It is an intricate chemical compound that belongs to the class of aromatic polyfunctional aldehydes <sup>[8]</sup>. An intriguing 2D polymer known as "graphimine," with an exceptionally rigid, triangular pore topology, was created by a plan wherein the monomer would, in the presence of acid, undergo a transimination reaction between the aldehyde and benzophenone imine groups on separate molecules, releasing the benzophenone protecting group in the process <sup>[9, 10]</sup>. A novel high-performance material known as "graphamid" was created by the hydrogen-bonded aromatic networks seen in poly(p-phenylene terephthalamide) (PPTA) <sup>[5, 9]</sup>. Graphamid is a 2D polymer that resembles a sheet and shares a chemical composition with PPTA <sup>[11]</sup>. It is made up of six adjacent benzene rings joined at each carbon by amide groups. The conjugated system combining the diphenylmethylene groups and the benzene core may give rise to intriguing photophysical characteristics in the molecule <sup>[9, 10, 12-14]</sup>. The potential applications of complex aromatic compounds extend to the development of advanced materials <sup>[9, 12, 15]</sup> such as organic semiconductors, light-emitting diodes (LEDs), and photovoltaic materials.

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Additionally, depending on their structure, these compounds could be utilized in chemical sensor technology and catalysis, serving as catalysts in organic reactions [16].

## 2. Computational detail

A computational quantum mechanical modeling technique called density functional theory is used to determine the electronic density at any point in paradigm and then utilize that data to look into the electronic structures of atoms and molecules [16-18]. Instead of wave functions, it relies on the idea of electron density. One particular function in the DFT framework is B3LYP. It consists of two parts (correlation and exchange): the correlation functional (VWN) introduced by Vosko, Wilk, and Nusair [19-21], the three-parameter Lee-Yang-Parr correlation functional (LYP), and the Becke exchange functional (B). Accurate results for a range of molecular systems, including excited and ground states, are intended to be produced using B3LYP [22-25]. By combining the benefits of DFT and Hartree-Fock (HF) theory, hybrid functionals contribute significantly to the field of computational chemistry and provide increased accuracy for a wide range of chemical applications. In summary, hybrid functionals are widely used, such as Quantum chemistry for predicting molecular geometries, vibrational frequencies, and reaction energies, and materials science for studying the properties of solids, surfaces, and nanomaterials. As well as; The frontier orbital energies are determined by the following relationship under Koopman's approximation [26-29]. Subsequently, electronegativity, hardness, softness, and electrophilicity can be determined based on the ionization potential (I.P.) and electron affinity (E.A.) values. According to the relationships following [28, 30-33]:

$$E_g = E_{LUMO} - E_{HOMO} \quad (1)$$

$$\left. \begin{aligned} I.P. &= -E_{HOMO} \\ E.A. &= -E_{LUMO} \end{aligned} \right\} \quad (2)$$

$$\chi = \frac{I.P.+E.A.}{2} \quad (3)$$

$$\eta = \frac{I.P.-E.A.}{2} \quad (4)$$

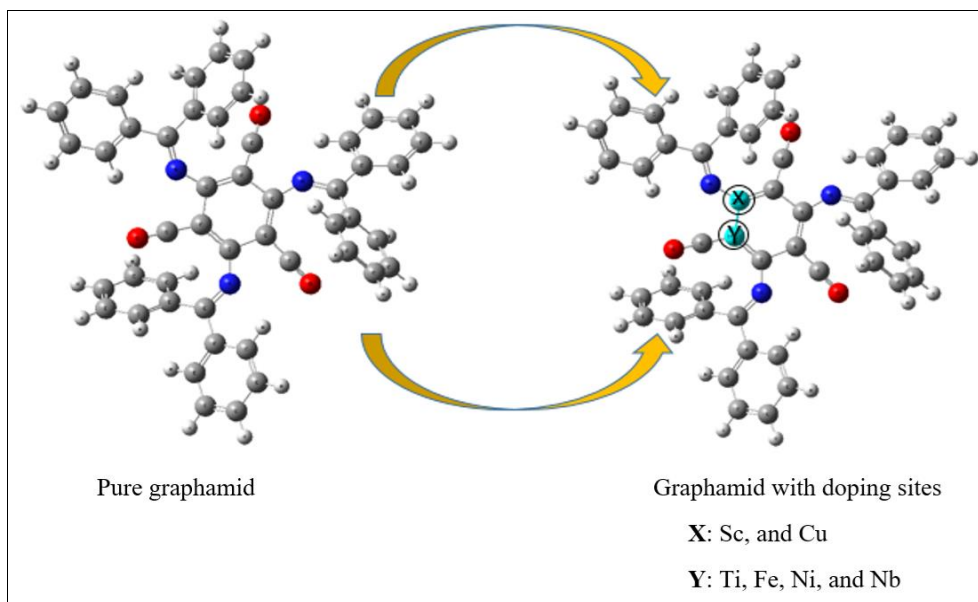
$$\sigma = \frac{1}{2\eta} \quad (5)$$

$$\omega = \frac{(I.P.+E.A.)^2}{4(I.P.-E.A.)} \quad (6)$$

## 3. Results and Discussion

2, 4, 6-Tris ((diphenylmethylene) amino) benzene-1, 3, 5-tricarbaldehyde (graphamid) is a complex organic compound classified under polyfunctionalized aromatic aldehydes. This compound features a benzene ring with aldehyde groups (-CHO) at positions 1, 3, and 5. At positions 2, 4, and 6, the benzene ring is substituted with diphenylmethylamino groups (-N=C(C6H5)2). A diphenylmethylene group (a central carbon bonded to two phenyl rings) attached to the nitrogen. The structure displays a degree of symmetry,

indicating it might be designed for interactions between atoms in chemical systems. The convergence of the optimization is evaluated using criteria such as the maximum force, root mean square (RMS) force, maximum displacement, and RMS displacement. Successful optimization meets all these criteria. During the optimization, the software calculates the total energy of the molecule at each step. The optimization proceeds until the changes in energy and geometry between iterations fall below predefined thresholds, indicating that a local minimum has been reached. In order to find the most stable configuration, this process entails moving atoms around to reduce the system's total energy. In this paper, we investigate the Density Functional Theory (DFT) method's geometry optimization of the structure 2,4,6-Tris((diphenylmethylene)amino)benzene-1,3,5-tricarbaldehyde (graphamid) utilizing the 6-31G(d) basis set and the B3LYP functional; as shown in figure 1. The absence of imaginary frequencies in the optimization results attests to the accuracy and correctness of the findings. Figure 1 purports to show a pure graphamid molecular structure, with the atoms of carbon, oxygen, nitrogen, and hydrogen represented by the gray, red, blue, and off white spheres, respectively. After the original structure (Graphamid) was optimized, i.e., it reached the lowest energy in the ground state. Utilizing atoms from the periodic table's transition metal region, the graphamid molecule was enhanced with these atoms at two distinct locations, denoted by the symbols X and Y, respectively, as shown in figure 1. The impurity X and the impurity Y each took the place of one carbon atom in the center ring. The atoms of copper (Cu) and scandium (Sc) are referred to as impurity X, whereas the atoms of titanium (Ti), iron (Fe), nickel (Ni), and niobium (Nb) are referred to as impurity Y. The Gaussian 09 software [35] was utilized for all geometric optimization of structural procedures, with the basis set 6-31G and the density functional theory DFT/B3LYP. All the energy values for HOMO and LUMO have a negative sign, which indicates that all the compounds are bonded. Various metal changes result in slightly varying HOMO energies. Of the structures in Table 1, the structure graphamid-Fe has the highest negative HOMO energy (-4.01565 eV), meaning that it is the most stable. When compared to other doped structures, graphamid-Ti has the least negative HOMO energy (-3.62818 eV), indicating a little less stability. LUMO energies also show variations depending on the atom doping of the metal. Graphamid-Cu has the most negative LUMO energy (-2.79447 eV), which could suggest higher electron affinity. and versus; the structure graphamid-Nb has the least negative LUMO energy (-2.25843 eV). The energy gap is an important parameter for determining the electronic properties of materials. Graphamid-Cu has the smallest energy gap (1.084046 eV), suggesting it may be the most conductive or have the highest reactivity among the listed structures. It might be useful in semiconductor applications where high conductivity is desired, such as solar cells, sensors, or transistors. Graphamid-Fe and graphamid-Nb have the largest energy gap (1.512876 eV) and 1.500087 eV, respectively, indicating they may be the least conductive or have lower reactivity compared to others. Their larger energy gaps suggest they could be used in situations where stability is more critical than conductivity, possibly in insulating layers, stable substrates, or catalytic materials.



**Fig 1:** pure graphamid structure and graphamid structure with doping sites

**Table 1:** The energies of the highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), and the energy gap ( $E_g$ ) for pure Graphamid and its doped structures with various metal elements.

All values are measured in electron volts (eV)			
Structure	$E_{HOMO}$	$E_{LUMO}$	$E_g$
Pure Graphamid	-3.8094	-2.47611	1.33329
Amid-Sc	-3.6709	-2.49189	1.179009
Amid-Ti	-3.62818	-2.26061	1.367575
Amid-Fe	-4.01565	-2.50278	1.512876
Amid-Ni	-3.84205	-2.40863	1.433423
Amid-Cu	-3.87851	-2.79447	1.084046
Amid-Nb	-3.75852	-2.25843	1.500087

From Table 2, it can be noted that graphamid titanium has the lowest I.P. value (3.628181 eV), which means it is the easiest to ionize among the listed systems. Graphamid-Fe has the highest I.P. value (4.015652 eV), which indicates it is the hardest to ionize and thus indicates a more stable electron configuration. Graphamid-Ti and graphamid-Nb have the lowest E.A. values (2.260607 eV and 2.25843 eV, respectively), which means they have a lower tendency to accept electrons compared to the other compounds. Copper amide has the highest E.A. value (2.794467 eV), which indicates that it has a high tendency to gain an electron. The balance between ionization potential and electron affinity is crucial in designing semiconductor materials. Compounds with appropriate I.P. and E.A. values can be tuned for specific electronic and optoelectronic applications. High-I.P. structures like graphamid-Fe are suitable for applications where material stability is critical. Structures with high electron affinity, such as graphamid-Cu, can be good candidates for catalysis due to their ability to accept electrons easily. Also, compounds with significant changes in I.P. and E.A. upon doping, for instance, graphamid with Fe and Ti,

can be used in sensors where sensitivity to electron gain or loss is crucial. The provided data in table 2 includes the wavelengths ( $\lambda$ ) in nanometers (nm) for various compounds, which likely correspond to the wavelengths of maximum absorption or emission. This transition from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO) can be related to these values in terms of electronic transitions within the molecules. Table 2 shows that the wavelength values of all compounds fall within the near-infrared region of the visible spectrum. By comparing tables 1 and 2, The relationship between the wavelength and the energy gap reinforces the electronic properties discussed previously. For instance, graphamid-Cu with the longest wavelength (smallest energy gap) correlates with its higher electron affinity and lower reactivity in terms of losing electrons. By understanding the relationship between wavelength and energy gap, these materials can be tailored for specific applications that require precise electronic and optical characteristics. therefore, These optical properties have significant implications for their potential applications in optoelectronics, photovoltaics, and biological fields.

**Table 2:** The ionization potential (I.P), electron affinity (E.A), and the wavelengths for graphamid and its derivatives with various metal elements.

Structure	I.P (eV)	E.A (eV)	$\lambda$ (nm)
Pure Graphamid	3.8094	2.47611	930.030226
Amid-Sc	3.670901	2.491892	1051.730733
Amid-Ti	3.628181	2.260607	906.7144398
Amid-Fe	4.015652	2.502776	819.6309546
Amid-Ni	3.842052	2.408629	865.0621624
Amid-Cu	3.878513	2.794467	1143.862899
Amid-Nb	3.758517	2.25843	826.6187228



The infrared spectrum's frequency is shown on the x-axis as wavenumbers ( $\text{cm}^{-1}$ ). The compound's molar absorptivity ( $\epsilon$ , in  $\text{M}^{-1} \text{cm}^{-1}$ ), which shows how strongly it absorbs IR light at each frequency, is represented by the y-axis on the left. A distinct scale ( $D$  in  $\text{esu}^2 \text{cm}^2$ ), represented by the y-axis on the right, may be related to the measurement of absorption intensity.

The appearance of new peaks next to the peaks present in the original compound is attributed to the vibration of bonds and atoms of impurity metals added to the original compound,

such as scandium, titanium, etc., as shown in Figure 2. Harvesting, the IR spectrum provides valuable insights into the vibrational modes and functional groups present in the compound. By analyzing the key peaks and their corresponding frequencies, one can infer the presence of specific bonds and structural features. This information, when combined with the electronic properties (I.P., E.A.) and optical data (wavelengths), offers a comprehensive understanding of the compound's characteristics and potential applications.

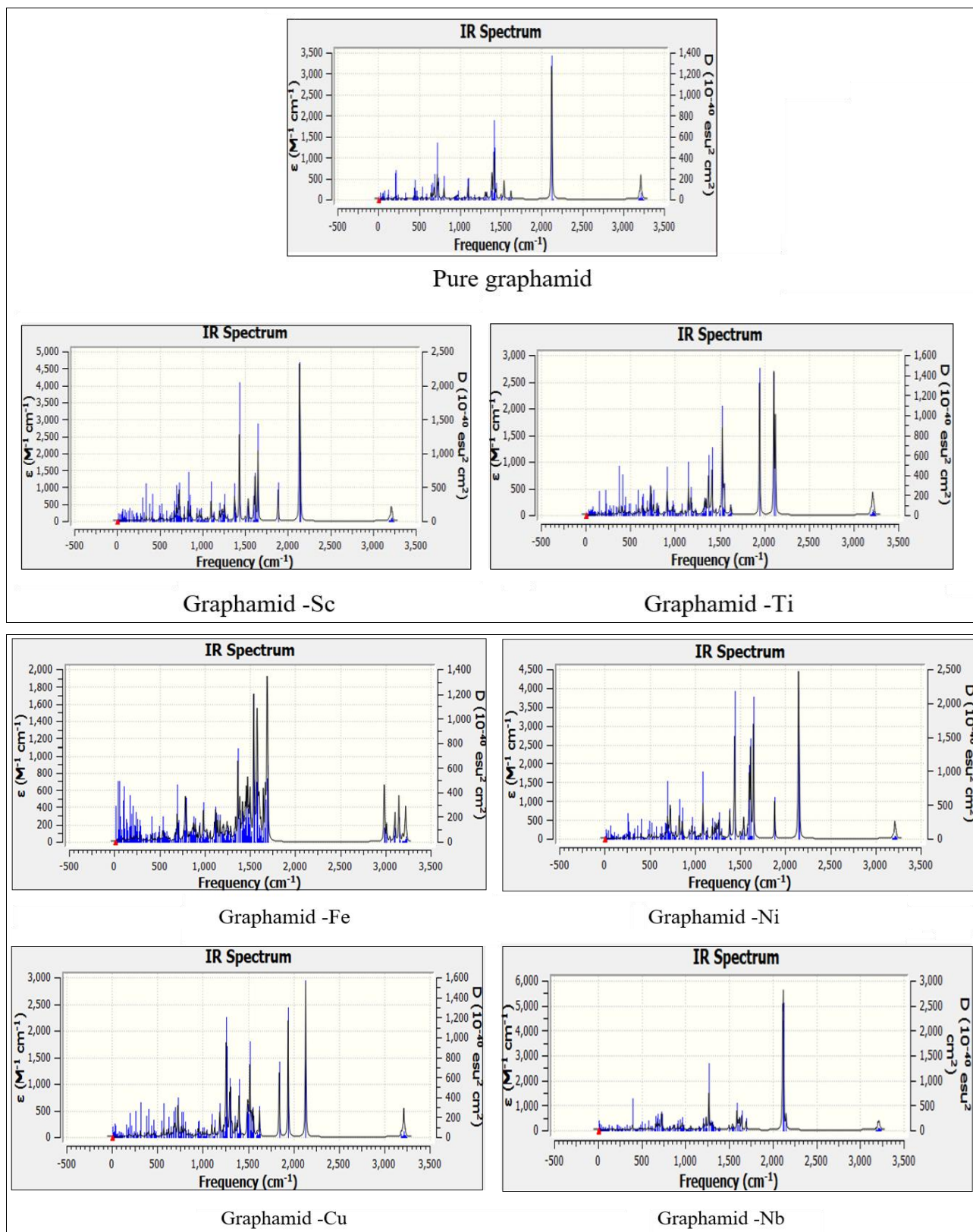
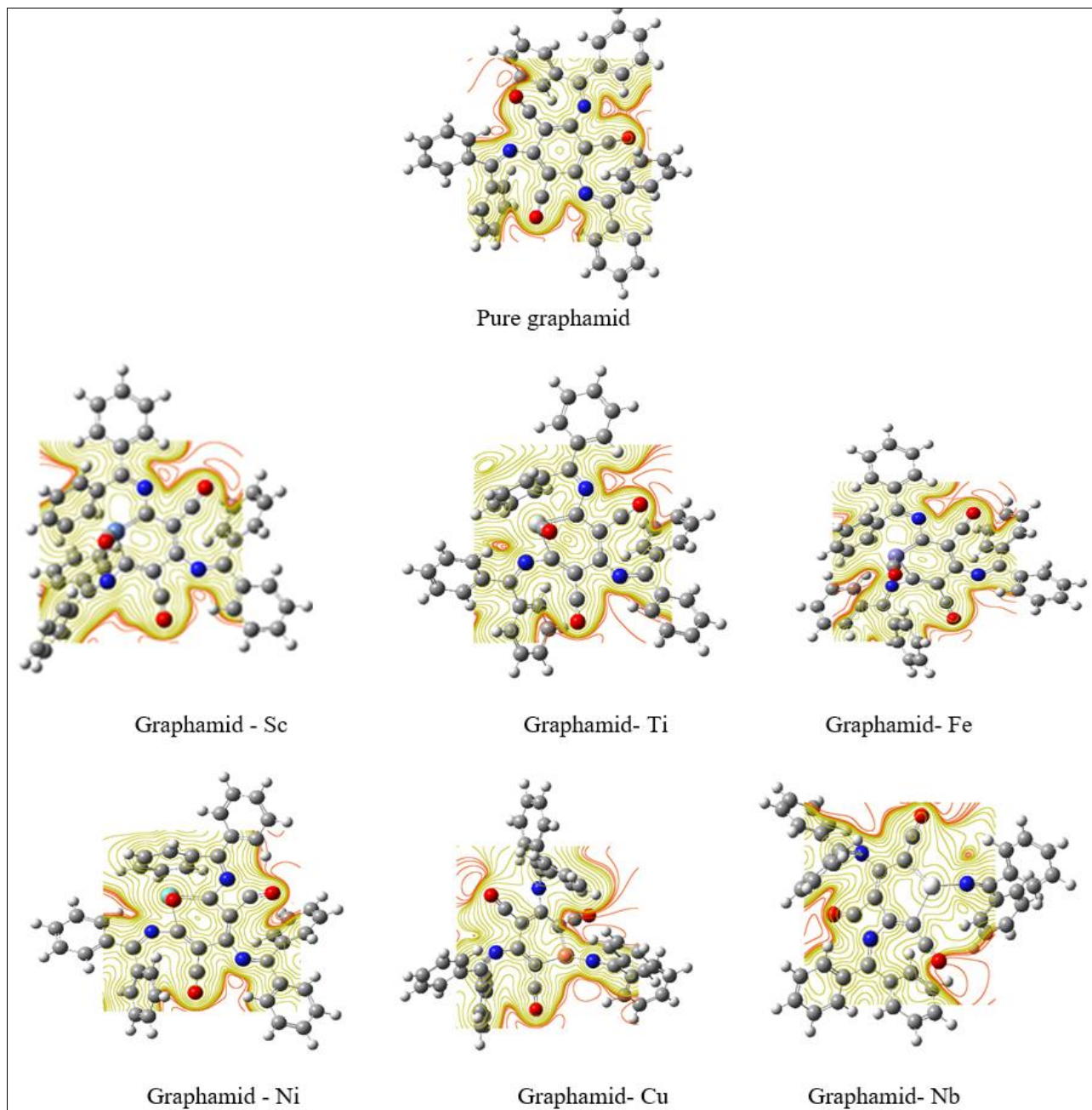


Fig 2: Infrared (IR) spectra of a pure and impure graphamid compounds



**Fig 3:** The pattern of electron distribution in the original compound and the other compounds.

It is noticeable that the contours in the central ring of the original compound are regular. This is attributed to the fact that the distribution of charges is regular, while when moving outward, there will be a clustering of charges that appears in red near the oxygen atoms. However, in the case of adding metal atoms (Sc, Ti, Fe, Ni, Cu, and Nb) to the central ring, i.e., after the doping process, the impurity of the metal atoms can change the distribution of electron density, and thus the regularity of the rings will be disturbed, which is evident from the contour curves around the metal sites. The extent of irregularity depends on the type of impurity. This affects the HOMO and LUMO levels and thus changes the ionization potential and electron affinity. Also, one of the things that can be observed in Figure 3 is that these rings represent Brillion regions, where the central ring of the contours represents the first Brillion region, the second ring represents the second Brillion region, and so on to the rest of the rings. And the electrons are bound to the region in which they are located and cannot move to another region unless they acquire energy greater than the forbidden energy between the two regions.

The values of electronegativity, hardness chemical, softness chemical, and electrophilicity can be derived by using equations 3-6. Then they are tabulated in Table 3. The least electronegativity, 2.944394 eV, occurs in the structure graphamid-Nb, indicating a comparatively weaker tendency to attract electrons. So, the maximum electronegativity (3.33649 eV) is observed in the structure of graphamid-Sc, suggesting a strong tendency to attract electrons. It can be deduced that the chemical hardness is inversely proportional to the chemical softness by comparing the values in Table 3 with the chemical hardness values in Table 3. Also, it can be concluded that the energy gap is directly proportional to the chemical hardness by comparing the energy gap values in Table 1 with the chemical hardness values in Table 3. This is because the largest energy gap value, such as graphamid-Fe 1.512876 eV, corresponds to the largest hardness value 0.756438 eV (at the lowest softness 0.660993 eV<sup>-1</sup>), indicating that it is less polarizable and more resistant to electronic deformation. In order to liberate the electron and get to the conduction level, additional energy is needed. In

contrast to the lowest energy gap value of the graphamid-Cu structure, the graphamid-Cu structure has the lowest hardness 0.542023 eV (at the highest softness 0.92247 eV<sup>-1</sup>). Which indicates that it is more polarizable and less resistant to electronic deformation. The best compounds that can be applied in sensors are graphamid-Cu and graphamid-Sc. This is due to the fact that both compounds have high reactivity. Which in turn can be attributed to the location of the impurity atoms in the compound, where the impurity site X was found to be more active and less stable than the impurity site Y, as shown in Figure 1. Both iron-doped and titanium-doped graphamid have stable structures and low reactivity, which means they can be used in catalytic applications or other uses. Finally, the structure of nickel-doped graphamid has balanced stability and reactivity, which is useful for applications requiring a compromise between these properties.

**Table 3:** The values of electronegativity, hardness chemical, softness chemical, and electrophilicity.

structure	$\chi$	$\eta$ (eV)	$\sigma$ (eV) <sup>-1</sup>	$\omega$
Pure Graphamid	3.142755	0.666645	0.750024	7.407923
Amid-Sc	3.33649	0.589505	0.84817	8.053375
Amid-Ti	3.259214	0.683787	0.731222	6.339293
Amid-Fe	3.081396	0.756438	0.660993	7.021378
Amid-Ni	3.008474	0.716711	0.697631	6.814287
Amid-Cu	3.125341	0.542023	0.92247	10.26909
Amid-Nb	2.944394	0.750044	0.666628	6.033591

Because of the smallness of other energies (vibrational energy and rotational energy) compared to electronic energy, the total energy can be expressed in terms of electronic energy, neglecting vibrational and rotational energy. Total energy indicates the stability of each structure. A higher total energy generally denotes a less stable structure. Greater stability is indicated by a lower total energy, which is important for materials used in structural applications where durability and stability are essential. The dipole moment measures the concentration of electric charge within the molecule or structure. Higher dipole moments stand for a greater separation of negative and positive charges. It is clear that the materials that have a dipole moments can be used in applications requiring electrical polarization, such as in piezoelectric devices, capacitors, or sensors where detecting changes in electric fields is necessary [35]. Polarizability reveals how easily the electron distribution within the structure can be distorted by an external electric field. Greater interaction with electromagnetic fields can be indicated by higher polarizability [36]. From Table 4, it can be noted that the values of the dipole moment of the original compound before doping were very small (0.577 Debye). While when adding impurity atoms, the values of the dipole moment increase, the largest value is for the compound after doping with copper atoms (9.884 Debye), and this can be attributed to the nature of the copper material, which is greatly affected by the distribution of charges, as is clear when compared with the values of the energy gap for the same compound in Table 1. Structure of graphamid-Cu, which has a high dipole moment and moderate polarizability. This combination of two parameters makes it potentially useful in applications such as electrical devices. Due to its high dipole moment, Amid-Cu could be used in capacitors or sensors where electrical polarization is advantageous. As well as optoelectronics applications. Its moderate polarizability suggests it could interact efficiently with electromagnetic fields, making it suitable for use in optoelectronic devices such as LEDs or

photovoltaic cells.

**Table 4:** The values of total energy (T.E.), dipole moment in debye unit, and Polarizability in atomic unit.

Structure	T.E. (hartree)	D.M. (debye)	Polarizability
Pure Graphamid	-2224.621	0.577	704.357
Amid-Sc	-2943.895	6.312	705.489
Amid-Ti	-3032.216	6.212	735.363
Amid-Fe	-3444.481	3.597	689.914
Amid-Ni	-3687.922	5.046	722.089
Amid-Cu	-3819.440	9.884	692.048
Amid-Nb	-5924.868	5.201	768.918

#### 4. Conclusions

2, 4, 6-Tris ((diphenylmethylene) amino) benzene-1, 3, 5-tricarbaldehyde is a polyfunctional aromatic compound with potential applications such as materials science, sensor technology, and catalysis. The electrical characteristics of graphamid are greatly impacted by the addition of different metals. Comprehending these alterations facilitates the customized development of materials for particular uses, capitalizing on the distinct characteristics bestowed by every alteration to metal. The wavelength values of all compounds fall within the near-infrared region of the visible spectrum. The energy gap is directly proportional to the chemical hardness. The best compounds that can be applied in sensors are graphamid doped with Cu and graphamid doped with Sc, and this is attributed to the fact that both compounds have high reactivity. Finally, structure graphamid-Cu which has a high dipole moment and moderate polarizability. it potentially useful in applications such as sensors or photovoltaic cells.

#### 5. Conflicts of interest

There are no conflicts to declare.

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