Molecular modeling analyses for the effect of solvents on amino acids

Article · October 2019

DOI: 10.33263/BRIAC95.379383

CITATION
1

READS
164

12 authors, including:

Ahmed M. Bayoumy
Ain Shams University
20 PUBLICATIONS **99** CITATIONS
SEE PROFILE

Sarah Abdelmoaty Elbiomy
Ain Shams University
1 PUBLICATION **1** CITATION
SEE PROFILE

Shimaa G. Elgabaly
cairo higher institute for engineering & computer science and management
4 PUBLICATIONS **4** CITATIONS
SEE PROFILE

Mohamed Gouda
Cairo University
22 PUBLICATIONS **46** CITATIONS
SEE PROFILE

Volume 9, Issue 5, 2019, 4379 - 4383 ISSN 2069-5837

Biointerface Research in Applied Chemistry

www.BiointerfaceResearch.com

https://doi.org/10.33263/BRIAC95.379383

Original Research Article Open Access Journal

Received: 21.08.2019 / Revised: 28.09.2019 / Accepted: 02.10.2019 / Published on-line: 08.10.2019

Molecular modeling analyses for the effect of solvents on amino acids

Ahmed M. Bayoumy [1], Rania Badry [2], Heba A. Gaber [3], Sarah A. Elbiomy [1], Shimaa G. El Gabaly [4], Mariam Sayed Abd ElAziz [5], Shrouk Mohamed Gouda [6], Hanan Elhaes [2], Ibrahim S. Yahia [7,8,9], Heba Y. Zahran[7,8,9], Medhat Ibrahim [10,*]

[1]Physics Department, Biophysics Branch, Faculty of Science, Ain Shams University, 11566, Cairo, Egypt
[2]Physics Department, Faculty of Women for Arts, Science and Education, Ain Shams University, 11757, Cairo, Egypt
[3]Biophysics and Laser Science Unit, Research Institute of Ophthalmology, 2 Al Ahram Str. 12111 Giza, Egypt
[4]Basic Science Department, Cairo Higher Institute for Engineering, Computer Science and Mangement, 11477-57 SB EG, Cairo, Egypt
[5]Biochemistry/Chemistry Program, Faculty of Science, Ain Shams University, 11566, Cairo, Egypt
[6]Applied Biotechnology Program, Faculty of Science, Ain Shams University, 11566, Cairo, Egypt
[7]Research Center for Advanced Materials Science (RCAMS), King Khalid University, Abha 61413, P.O. Box 9004, Saudi Arabia
[8]Advanced Functional Materials & Optoelectronic Laboratory (AFMOL), Department of Physics, Faculty of Science, King Khalid University, P.O. Box 9004, Abha, Saudi Arabia
[9]Nanoscience Laboratory for Environmental and Bio-Medical Applications (NLEBA), Semiconductor Lab., Metallurgical Lab. 2 Physics Department, Faculty of Education, Ain Shams University, Roxy, 11757 Cairo, Egypt
[10]Spectroscopy Department, National Research Centre, 33 El-Bohouth Str. 12622 Dokki, Giza, Egypt
*corresponding author e-mail address: ***medahmed6@yahoo.com*** | Scopus ID 8641587100

ABSTRACT

Influence of solvation with various solvents is a vital issue for several applications of amino acids. Considering the impact of solvents and many other factors is an important point of research to get much more accurate data on their behavior. Hence, molecular modeling calculations were conducted for some amino acids in both cases; gaseous state and under the effect of several solvents; DMSO, acetonitrile, nitromethane, and methanol. DFT was utilized at B3LYP theoretical level and 6-31G(d,p) as a basis set. Geometrical parameters of both amino and carboxyl terminals were studied. Resulting data ascertain that various solvation processes impact the interested parameters that have to be considered for further applications.

Keywords: *Amino acids; Histidine; Arginine; Solvation; DFT; Geometrical parameters.*

1. INTRODUCTION

Livings composed of several macromolecules; carbohydrates, proteins, nucleic acids, and lipids. Proteins are treated as one of the most vital macromolecules where they carry out many vital processes. They may be found in the form of receptors, enzymes, signaling compounds, hormones, structural units of muscles and many other roles. Proteins are comprised of several polypeptide chains. Polypeptides have vital applications in our living bodies and in various scientific fields [1]. They contain hundreds of smaller entities called amino acids. Amino acids are the main structural and functional units of proteins. Twenty different amino acids present in all living organisms. They all share the same chemical structure where they all composed of a central alpha carbon atom linked to four entities; hydrogen atom, carboxyl group (C-terminal), amino group (N-terminal) and R-group, by single sigma covalent bonds. Twenty different alkyl groups yield 20 different amino acids. There are many aspects for classifying amino acids such as their chemical structure, their physical properties, chemical features, and nutritional requirements. Regarding the last aspect, they can be categorized into essential and nonessential amino acids. Methionine is one of the essential amino acids. It is one of the amino acids, besides cysteine, that has sulfur element in their R side-chain structure. Methionine (abbreviated as Met or M) has an amino group (which is protonated NH_3^+ under biological conditions), carboxylic acid group (which is deprotonated COO^- under biological conditions), and an S-methyl thioether side chain. It is usually classified as an aliphatic nonpolar amino acid. It plays unique roles in protein structure and metabolism. Methionine is usually involved in growth control processes by indicating the start of the coding region and it is the first amino acid produced in a nascent polypeptide during mRNA translation. Methionine had been used in pharmaceuticals and biological applications for many decades and reported as effective corrosion inhibitors in different aggressive media for copper, aluminum, and others [2]. On the same manner, arginine is the same as methionine in being one of the essential amino acids [3]. It is usually converted in the body into nitric oxide directly by the aid of nitric oxide synthase enzyme. Arginine is a popular supplement for athletes as it is touted to increase nitric oxide activity in the body [4]. It is characterized by its high flexibility that can be attributed to its existence in the zwitter-ionic form, hence it contributes in the coordination with body salts through various interaction types such as hydrogen bonds and ionic bonds [5]. Therefore, arginine amino acid can undergo many conformational changes. Critical changes in metabolism processes of arginine that lead to a drop in its intracellular concentration [6, 7]. However, raising its levels in the body leads to induction of various global metabolic variations including a change from glycolysis to oxidative phosphorylation in activated T cells and stimulating the generation of central memory-like cells endowed with higher survival capacity in antitumor activity [8]. Activation of T cells consumes large amounts of glucose, fatty acids, and amino acids. Concentrations

of L- arginine in cells affect directly the metabolic fitness as well as the survival capacity of T cells that are crucial for anticancer response [9-11]. Unlike both methionine and arginine, tyrosine is one of the non-essential amino acids. It is usually found in several foods and drinks such as chicken, milk, cheese, almonds, peanuts, milk and many more. It is produced from dietary proteins such as salami and those that are aged, in particular, red wine and most types of cheese [12]. Tyrosine is one of the effective anti-depressant agents which, in addition, enhance the action of immune system in livings' bodies [13]. It is one of the most frequently found amino acids in building up all types of proteins. Furthermore, it is common in improving memory, alertness, and learning specifically in stressful cases [14]. Tyrosine is the precursor amino acid for numerous neurotransmitters where it raises their blood level [15]. It is the It is usually utilized in sending chemical signals to the brain in several circumstances such as mental alertness. It is the precursor of dopamine neurotransmitter. Histidine amino acid was proven to be essential for all of the infants, normal adults and those suffering from uremia [16, 17]. It is one of the aromatic amino acids that is abundantly found in blood hemoglobin. Moreover, its nitrogen atom acts as an electron donor during the building processes of bonds including electron-poor atoms and it is also very important for plant growth and development [18]. Histidine, rather than other amino acids, play versatile roles in formulating structure and function of proteins [19-21]. This can be attributed to its unique side chain that composed of imidazole aromatic motif [22].

Conducting molecular modeling at various theoretical levels could be useful in understanding the chemical as well as structural features of amino acids and several structures and compounds as well [23-25]. Its concepts were greatly utilized in order to understand the interaction mechanism between chitosan and some amino acids [26]. Furthermore, they were conducted to investigate the impact of Hydrated Dioxin on both physical as well as geometrical parameters of amino acids [27]. These concepts were utilized also to study the influence of alkaline elements on the structural and electronic features of Glycine amino acid [28] and to investigate the interaction between aspartic acid and iron element [29]. In addition, it is also reported that calculations of molecular modeling always confirm the experimental data and introduce a reasonable way to understand important issues in all of the biological, chemical and environmental points of research [30-32]. Therefore and based upon the reported importance of molecular modeling, the present work is carried out to clarify the effect of solvation processes on the geometrical parameters of some amino acids using DFT level of theory.

2. MATERIALS AND METHODS

Calculation details.

Molecular models of some amino acids; methionine, arginine, tyrosine, and histidine, were built up and energy calculations were performed using GAUSSIAN 09 software which is implemented at Spectroscopy Department, National Research Centre (NRC) [33]. The calculations were conducted via Density Functional Theory (DFT) level at Becke-style 3-Parameter Density Functional Theory (using the Lee-Yang-Parr correlation functional) (B3LYP) [34-36] and 6-31g(d,p) as a basis set. Geometrical parameters of the built-up amino acids were studied in two states; gaseous state and under solvation with various solvents, for example, dimethylsulfoxide (DMSO), nitromethane (NM), acetonitrile (AN) and methanol (Meth).

3. RESULTS

3.1. Building up model molecules.

Four amino acids as well as other two aromatic ones, up as shown in figure 1. Two aliphatic amino acids, as well as the other two aromatic ones, were chosen for this study. They all possess the same chemical architecture with central alpha carbon atom linked to four moieties including hydrogen atom, carboxyl group (C-terminal), amino group (N-terminal) and alkyl group, by single covalent bonds.

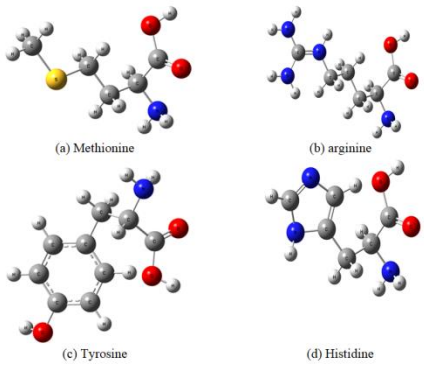

Figure 1. Model molecules of the four built-up amino acids (a) methionine, (b) arginine, (c) tyrosine, and (d) histidine.

Methionine is the only built up molecule; that has a sulfur element, in its R group, which is surrounded by two methyl groups. Such sulfur atom enables methionine from making S-S bridges with other protein chains. Arginine is one of the basic amino acids since it contains three amine groups in its alkyl side chain. Such a structure enhances its positivity when placed in an alkaline media. Tyrosine is one of the aromatic amino acids where its side chain is composed of a terminal phenol structure that linked to the alpha central carbon atom through a methyl group. On the same manner, histidine has an aromatic structure. Its alkyl chain contains imidazole aromatic motif bonded to the alpha carbon by a methyl group via single covalent bond.

3.2. Energy calculations.

Energy calculations were conducted for the studied amino acids through DFT calculations using the B3LYP hybrid theoretical level and 6-31G(d,p) as our basis set. The calculations were carried out for the interesting amino acids in two cases; gaseous state and under solvation with various solvents, for example DMSO, nitromethane (NM), acetonitrile (AN) and methanol (Meth). Furthermore, geometrical parameters were studied in all cases. **Table 1** illustrates the resulting geometrical parameters of the interested structures where both bond lengths and bond angles of C and N terminals of the investigated structures were

considered. Solvation of amino acids with various solvents seem to affect the geometrical parameters of their terminals, as illustrated in table 1, which should be considered in further applications. For methionine amino acid, solvation with DMSO has no impact on the interested geometrical parameters except for the length of the C-O bond which is lowered from 1.4300 to 1.3013 A, and the bond angle named HOC where it is increased from 109.4712^{o} to 120.00^{o}. However, both nitromethane and acetonitrile solvents have significant effect on all the studied parameters. Both of them cause the increment of the length of the two NH bonds as well as the OH one, and the OCO angle. It is obvious that the increment results from nitromethane are higher than that of acetonitrile. Similarly, both lower the other geometrical parameters where the length of both C=O and C-O bonds and the angles HNH and HOC are decreased. On the same manner of DMSO, methanol has no impact on the parameters of methionine except for HNH bond which is raised greatly from 109.4712^{o} to 120.00^{o}. Resulting data of tyrosine amino acid seem to be different from those of other amino acids where they all have the same effect on the studied parameters to nearly the same extent. They all cause the increasing of lengths of the two NH bonds, C=O and OH bonds, and the angles named HOC and OCO. However, they lead to the lowering of the CO bond length and HNH bond angle. Similarly, solvation of histidine with different amino acids has the same behavior, as previously explained for tyrosine, but with different ratios. Nitromethane has the greatest effect among the studied solvents in both cases of increment or decrement of interesting parameters. Both acetonitrile and methanol have typical effects on the studied parameters. Regarding arginine, it can be noticed that different solvents have various impacts on the studied parameters. They all have little effect on the two NH bonds. Furthermore, they have a greater decreasing impact on the HNH and OCO bond angles. However, they cause the increment of both C=O bond length and HOC bond angle. Methanol has the greatest effect with respect to other solvents. DMSO, acetonitrile, and methanol increase the C-O bond length, in contrary to nitromethane which decreases it. In addition, DMSO, nitromethane, and methanol lower the OH bond length, in contrast to acetonitrile that raises it from 0.9732A to 0.9780A.

Table 1. Geometrical parameters of C and N terminals of methionine (Met), tyrosine (Tyr), arginine (Arg) and histidine (His) amino acids in the gaseous state and under solvation with DMSO, nitromethane (NM), acetonitrile (AN) and methanol (Meth) solvents calculated at DFT using B3LYP/6-31G(d,p) level.

		Amino group			Carboxyl group				
Amino Acid	**Solvation**	**NH(1)**	**NH(2)**	**HNH**	**C=O**	**CO**	**OH**	**HOC**	**OCO**
Met	**No Solvation**	1.0000	1.0000	109.4712	1.2584	1.4300	0.9600	109.4712	120.0000
	DMSO	1.0000	1.0000	109.4712	1.2584	1.3013	0.9600	120.0000	120.0000
	NM	1.0225	1.0224	106.3477	1.2178	1.3409	0.9939	108.1221	123.4966
	AN	1.0171	1.0169	106.9229	1.2148	1.3473	0.9735	107.3039	122.5548
	Meth	1.0000	1.0000	120.0000	1.2584	1.4300	0.9600	109.5000	120.0000
Tyr	**No Solvation**	1.0184	1.0171	107.3153	1.2137	1.3467	0.9733	106.3622	123.1507
	DMSO	1.0190	1.0180	106.3337	1.2162	1.3442	0.9743	107.4921	123.1728
	NM	1.0190	1.0180	106.3435	1.2162	1.3441	0.9743	107.4796	123.1780
	AN	1.0190	1.0180	106.3426	1.2162	1.3441	0.9743	107.4826	123.1806
	Meth	1.0190	1.0180	106.3454	1.2162	1.3441	0.9743	107.4787	123.1778
Arg	**No Solvation**	1.0204	1.0133	111.3940	1.2119	1.3522	0.9732	106.1330	122.7890
	DMSO	1.0205	1.0130	111.2810	1.2550	1.3466	0.9711	108.3210	121.2570
	NM	1.0205	1.0130	111.3210	1.2584	1.4300	0.9600	106.3130	122.0240
	AN	1.0207	1.0131	111.2940	1.2855	1.3410	0.9780	109.4150	120.0570
	Meth	1.0207	1.0128	111.1240	1.3013	1.3013	0.9669	109.8760	120.0110
His	**No Solvation**	1.0156	1.0171	107.9380	1.2125	1.3485	0.9726	106.4610	122.6390
	DMSO	1.0170	1.0175	106.7800	1.2159	1.3432	0.9737	107.2730	122.8170
	NM	1.0220	1.0207	106.2950	1.2190	1.3374	0.9935	107.8680	123.1620
	AN	1.0178	1.0189	106.3680	1.2149	1.3451	0.9743	107.5780	123.2830
	Meth	1.0178	1.0189	106.3740	1.2149	1.3451	0.9743	107.5740	123.2850

4. CONCLUSIONS

Molecular modeling calculations at DFT level were conducted for some interesting amino acids in two cases; gaseous state and under the influence of several solvation processes using diverse solvents; DMSO, AN, NM and Meth. DFT was carried out at the B3LYP theoretical level using 6-31G(d,p) basis set. Geometrical parameters of both amino and carboxyl terminals were studied. The conducted solvation processes ensure that solvation processes should be considered for future applications. Selecting a suitable solvent is an important point of research when starting a new investigation to eliminate the effect of solvents and get more accurate results. DFT proved to be a powerful tool to study amino acids which is in good agreement with the previous findings [37-43].

5. REFERENCES

1. Moudgil, L.; Jaiswal, J.; Mittal, A.; Saini, G.S.S.; Singh, G.; Kaura, A. Understanding the mechanism of adsorption of CTAB and polylysine on silver nanoparticles and detection of Hg^{2+}: Experimental and DFT study. *J Mol Liq* **201**9, *276*, 910–918, https://doi.org/10.1016/j.molliq.2018.12.106.

2. Khaled, K.F. Corrosion control of copper in nitric acid solutions using some amino acids – A combined experimental and theoretical study. *Corros. Sci.* **2010**, *52*, 3225-3234, https://doi.org/10.1016/j.corsci.2010.05.039.

3. Zyss, J.; Nicoud, J.F.; Coquillay, M. Chirality and hydrogen bonding in molecular crystals for phase-matched second-

harmonic generation: N-(4-nitrophenyl)-(L)-prolinol (NPP). *J Chem Phys* **1984**, *81*, 4160-4167, https://doi.org/10.1063/1.448134.

4. Nicoud, J.F.; Twieg, R.J. *Nonlinear Optical Properties of Organic Molecules and Crystals.* Academic Press, London, 1987.

5. Shkir, M.; Riscob, B.; Bhagavannarayana, G. Synthesis, growth, structural, spectroscopic, crystalline perfection, second harmonic generation (SHG) and thermal studies of 2-aminopyridinium picrate (2APP): A new nonlinear optical material. *Solid State Sci*. **2012**, *14*, 773-776, https://doi.org/10.1016/j.solidstatesciences.2012.04.022.

6. Shakir, M.; Kushawaha, S.K.; Maurya, K.K.; Kumar, S.; Wahab, M.A.; Bhagavannarayana, G. Enhancement of built-up generation, optical and dielectric properties in l-asparagine monohydrate single crystals due to an improvement in crystalline perfection by annealing. *J Appl Cryst* **2010**, *43*, 491-497, https://doi.org/10.1107/S0021889810008745.

7. Shkir, M.; Riscob, B.; Hasmuddin, M.; Singh, P.; Ganesh, V.; Wahab, M.A.; Dieguez, E.; Bhagavannarayana, G. Optical spectroscopy, crystalline perfection, etching and mechanical studies on P-nitroaniline (PNA) single crystals. *Opt Mater* **2014**, *36*, 675-681, http://dx.doi.org/10.1016/j.optmat.2013.11.009.

8. Ledoux, I.; Badan, J.; Zyss, J.; Migus, A.; Hulin, D.; Etchepare, J.; Grillon, G.; Antonetti, A. Generation of high-peak-power tunable infrared femtosecond pulses in an organic crystal: application to time resolution of weak infrared signals. *J Opt Soc Am B* **1987**, *4*, 987-997, https://doi.org/10.1364/JOSAB.4.000987.

9. Alves, N.L.; Derks, I.A.; Berk, E.; Spijker, R.; van Lier, R.A.; Eldering, E. The Noxa/Mcl-1 axis regulates susceptibility to apoptosis under glucose limitation in dividing T cells. *Immunity* **2006**, *24*, 703–716, https://doi.org/10.1016/j.immuni.2006.03.018.

10. Araki, K.; Turner, A.P.; Shaffer, V.O.; Gangappa, S.; Keller, S.A.; Bachmann, M.F.; Larsen, C.P.; Ahmed, R. mTOR regulates memory CD8 T-cell differentiation. *Nature* **2009**, *460*, 108–112, https://doi.org/10.1038/nature08155.

11. Bellone, M.; Cantarella, D.; Castiglioni, P.; Crosti, M.C.; Ronchetti, A.; Moro, M.; Garancini, M.P.; Casorati, G.; Dellabona, P. Relevance of the tumor antigen in the validation of three vaccination strategies for melanoma. *J Immunol* **2000**, 165, 2651–2656, https://doi.org/10.4049/jimmunol.165.5.2651.

12. Yadav, R.A.; Dixit, V.; Yogesh, M.**;** Santhosh, C. **(2015)** Raman and IR Spectral and DFT Based Vibrational and Electronic Characterization of Isolated and Zwitterionic Forms of L-Tyrosine. *Pharm Anal Acta* **2015**, *6*, 1-18, http://dx.doi.org/10.4172/2153-2435.1000439.

13. Hamedania, S.; Moradib, S. Molecular structure and DFT molecular orbital calculations of amino acid Tyrosine Proceedings of 5th International Congress on Nanoscience & Nanotechnology (ICNN2014), 2014.

14. De Armond, P.D.; Dietzen, D.J.; Pyle-Eilola, A.L. Amino acids disorders. In: *Biomarkers in Inborn Errors of Metabolism, Clinical Aspects and Laboratory Determination,* 1st Edition Garg, U., and Smith, L.D., Elsevier, 2017; pp. 35–40, https://doi.org/10.1016/B978-0-12-802896-4.00003-1.

15. Kopple, J.D.; Swendseid, M.E. Evidence that Histidine is an Essential Amino Acid in Normal and Chronically Uremic Man. *The Journal of Clinical Investigation* **1975**, *55*, 881-891, https://doi.org/10.1172/JCI108016.

16. Eagle, H. Amino acid metabolism in mammalian cell cultures. *Science* **1959**, *130*, 432-437, https://doi.org/10.1126/science.130.3373.432.

17. Ingle, R.A. Histidine biosynthesis. *Arabidopsis book* **2011**, *9*, 141, https://dx.doi.org/10.1199%2Ftab.0141.

18. Martínez, A. Evidence for a functionally important histidine residue in human tyrosine hydroxylase. *Amino Acids* **1995**, *9*, 285–292, https://doi.org/10.1007/BF00805959.

19. Uchida, K. Histidine and lysine as targets of oxidative modification. *Amino Acids* **2003**, *25*, 249–257, https://doi.org/10.1007/s00726-003-0015-y.

20. Remko, M.; Fitz, D.; Rode, B.M. Effect of metal ions (Li^+, Na^+, K^+, Mg^{2+}, Ca2+, Ni^{2+}, Cu^{2+} and Zn^{2+}) and water coordination on the structure and properties of l-histidine and zwitterionic l-histidine. *Amino Acids* **2010**, *39*, 1309–1319, https://doi.org/10.1007/s00726-010-0573-8.

21. Li, F.; Fitz, D.; Fraser, D.G.; Rode, B.M. Catalytic effects of histidine enantiomers and glycine on the formation of dileucine and dimethionine in the saltinduced peptide formation reaction. *Amino Acids* **2010**, *38*, 287–294, https://doi.org/10.1007/s00726-009-0249-4.

22. Liao, S.M.; Du, Q.S.; Meng, J.Z.; Pang, Z.W.; Huang, R.B. The multiple roles of histidine in protein interactions. *Chem Cent J* **2013**, *7*, 44, https://doi.org/10.1186/1752-153X-7-44.

23. Maddah, M.; Maddah, M.; Peyvandi, K. Molecular Dynamics Simulation of Methane Hydrate Formation in Presence and Absence of Amino Acid Inhibitors. *J Mol Liq* **2018**, *269*, 721-732, https://doi.org/10.1016/j.molliq.2018.08.108.

24. Ferreira, L.A.; Uversky, V.N.; Zaslavsky, B.Y. Effects of Amino Acids on Solvent Properties of Water. *J Mol Liq* **2019**, *277*, 123-131, https://doi.org/10.1016/j.molliq.2018.12.071.

25. Tang, H.; Ma, F.; Zhao, D.; Xue, Z. *Process Biochem* **2019**, *78*, 178-188, https://doi.org/10.1016/j.procbio.2019.01.011.

26. Abdel-Gawad, A.; Ibrahim, M. Spectroscopic Analyses of Chitosan Interactions with Amino acids. *J Comput Theor Nanosci* **2012**, *9*, 1120-1124, https://doi.org/10.1166/jctn.2012.2154.

27. Atta, D.; Gomaa, F.; Elhaes, H.; Ibrahim, M. Effect of Hydrated Dioxin on the Physical and Geometrical Parameters of Some Amino Acids. *J Comput Theor Nanosci* **2017**, *14*, 2405–2408, https://doi.org/10.1166/jctn.2017.6840.

28. Badry, R.; Omar, A.; Mohammed, H.; Mohamed, D.A.A.; Elhaes, H.; Refaat, A.; Ibrahim, M. Effect of Alkaline Elements on the Structure and Electronic properties of Glycine. *Biointerface Res Appl Chem* **2018**, *8*, 3682-3687.

29. Mahmoud, A.A.; Osman, O.; Elhaes, H.; Ferretti, M.; Fakhry, A.; Ibrahim, M.A. Computational Analyses for the Interaction between Aspartic Acid and Iron. *J Comput Theor Nanosci* **2018**, *15*, 470–473, https://doi.org/10.1166/jctn.2018.7113.

30. Abdelsalam, H.; Saroka, V.A.; Ali, M.; Teleb, N.H.; Elhaes, H.; Ibrahim, M.A. Stability and Electronic Properties of Edge Functionalized Silicene Quantum Dots: A First Principles Study. *Physica E: Low-dimens Syst Nanostruct* **2019**, *108*, 339–346, https://doi.org/10.1016/j.physe.2018.07.022.

31. Galal, A.M.F.; Atta, D.; Abouelsayed, A.; Ibrahim, M.A.; Hanna, A.G. Configuration and Molecular Structure of 5-Chloro-N-(4-sulfamoylbenzyl) Salicylamide Derivatives. *Spectrochim Acta* **2019,** *A 214*, 476–486, https://doi.org/10.1016/j.saa.2019.02.070.

32. Abdelsalam, H.; Teleb, N.H.; Yahia, I.S.; Zahran, H.Y.; Elhaes, H.; Ibrahim, M.A. First Principles Study of the Adsorption of Hydrated Heavy Metals on Graphene Quantum Dots. *J Phys Chem Solids* **2019**, *130*, 32-40, https://doi.org/10.1016/j.jpcs.2019.02.014.

33. Frisch, M.; Trucks, G.; Schlegel, H.; Scuseria, G.; Robb, M.; Cheeseman, J.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H.; Izmaylov, A.; Bloino, J.; Zheng, G.; Sonnenberg, J.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.;

Nakajim, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J.; Peralta, J. Jr.; Ogliaro, F.; Bearpark, M.; Heyd, J.; Brothers, E.; Kudin, K.; Staroverov, V.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J.; Iyengar, S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J.; Klene, M.; Knox, J.; Cross, J.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R.; Yazyev, O.; Austin, A.; Cammi, R.; Pomelli, C.; Ochterski, J.; Martin, R.; Morokuma, K.; Zakrzewski, V.; Voth, G.; Salvador, P.; Dannenberg, J.; Dapprich, S.; Daniels, A.; Farkas, O.; Foresman, J.; Ortiz, J.; Cioslowski, J.; Fox, D.; Gaussian; Inc.; Wallingford CT. Gaussian 09, Revision C.01. 2010.

34. Becke, A.D. Density-functional thermochemistry. III. The role of exact exchange. *The J Chem Phys* **1993**, *98*: 5648-5652, https://doi.org/10.1063/1.464913.

35. Lee, C.; Yang, W.; Parr, R.G. Development of the Colic-Salvetti correlation-energy formula into a functional of the electron density. *Phys Rev B* **1988**, *37*, 785-789, https://doi.org/10.1103/PhysRevB.37.785.

36. Vosko, S.H.; Wilk, L.; Nusair, M. Accurate spin-dependent electron liquid correlation energies for local spin density calculations: a critical analysis. *Can J Phys* **1980**, *58*, 1200-1211, https://doi.org/10.1139/p80-159.

37. Ashassi-Sorkhabi, H.; Moradi-Alavian, S.; Esrafili, M D.; Kazempour, A. " Hybrid sol-gel coatings based on silanes-amino acids for corrosion protection of AZ91 magnesium alloy: Electrochemical and DFT insights", Progress in Organic Coatings, **2019**, 131, 191-202. https://doi.org/10.1016/j.porgcoat.2019.01.052.

38. Al-Ahmary, K M.; Habeeb, M M.; Aljahdali, S H.; "Synthesis, spectroscopic characterization and DFT/TD-DFT computations of a novel charge transfer complex via hydrogen bonding between 3-amino-1,5-dimethylpyrazole with chloranilic acid in different solvents", Journal of Molecular Structure, 2019, 1181, 48-60 https://doi.org/10.1016/j.molstruc.2018.12.046.

39. Al-Ahmary, KM.; Al-Enezi, MS.; Habeeb, MM.; Spectroscopic characterisation and structural modelling of new hydrogen-bonded charge transfer complex between picric acid and 3-aminoquinoline", Phys. Chem. Liq., **2018**, 56 (1) 110-123. https://doi.org/10.1080/00319104.2017.1303834.

40. Hassen, S.; Chebbi, H.; Zid, M F.; Arfaoui, Y., "Assembly and weak interactions in the crystal structure of 2-amino-4-(3-bromophenyl)-1,3,5-triazinobenzimidazolium chloride studied by X-ray diffraction, vibrational spectroscopy, Hirshfeld surface analysis and DFT calculations", Journal of Molecular Structure, **2019**, 1179, 678-684 https://doi.org/10.1016/j.molstruc.2018.11.054.

41. Tamer, Ö.; Tamer, S A.; İdil, Ö.; Avcı, D.; Vural, H.; Atalay, Y. "Antimicrobial activities, DNA interactions, spectroscopic (FT-IR and UV-vis) characterizations, and DFT calculations for pyridine-2-carboxylic acid and its derivates", J. Mol. Struct., **2018**, 1152, 399-408. https://doi.org/10.1016/j.molstruc.2017.09.100.

42. Govindhan, R.; Karthikeyan, B. Nano Cu interaction with single amino acid tyrosine derived self-assemblies; study through XRD, AFM, confocal Raman microscopy, SERS and DFT methods Journal of Physics and Chemistry of Solids, **2017**, 111, 123-134. https://doi.org/10.1016/j.jpcs.2017.07.025.

43. Georgieva, S.; Todorov, P.; Bezfamilnyi, A.; Georgiev, A. Coordination behavior of 3-amino-5,5′-dimethylhydantoin towards Ni(II) and Zn(II) ions: Synthesis, spectral characterization and DFT calculations", Journal of Molecular Structure, 2018, 1166, 377-387 https://doi.org/10.1016/j.molstruc.2018.04.064

6. Acknowledgment

The authors are grateful to The Research Center for Advanced Material Science (RCAMS) at King Khalid University, with grant number (RCAMS/KKU/001-19).