Journal of
Composites Science

MDPI

Article

Computational-Simulation-Based Behavioral Analysis of Chemical Compounds

Pushpalatha Rajendran [1], Ramadevi Rathinasabapathy [2,*], Somasundaram Chandra Kishore [2] and Stefano Bellucci [3,*]

[1] Department of Electronics and Communications Engineering, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences (SIMATS), Saveetha University, Chennai 602105, India
[2] Department of Biomedical Engineering, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences (SIMATS), Saveetha University, Chennai 602105, India
[3] INFN-Laboratori Nazionali di Frascati, 00044 Frascati, Italy
* Correspondence: rama.adarsh09@gmail.com (R.R.); stefano.bellucci@lnf.infn.it (S.B.)

Abstract: This research focuses on obtaining the behavior of chemical compounds with respect to their molecular weight and optimization energy based on the variation in properties in organic carbon links. Here, behavioral analysis of compounds is used in the application of a metal organic framework to denote the high-grade compounds. The grade was selected based on the essential measure of optimization energy and molecular weight, and in turn, depicts the stability of material. Computation of the optimization energy and molecular weight of chemical compounds was performed with Avogadro software. Several force fields can be considered to compute optimized energy. Exclusively, three force fields, namely, the Universal Force Field (UFF), the General Amber Force Field (GAFF), and the Ghemical force field (Ghemical) were selected from Avogadro as these were more relevant to compounds considered in this research. The various chemical compounds examined in this work are Aluminum (Al), Boron (Br), Calcium (Ca), Chlorine (Cl), Indium (In), Potassium (K), Scandium (Sc), Silicon (Si), and Tungsten (W). Hence, molecular modeling of different compounds incorporated with three different force fields was evaluated in this work. In this study, we found that the In structure has more energy reduction, of 22.673 kJ mol^{-1} in UFF, when compared with the other two force fields. Thus, In has higher potential with more stability.

Keywords: Avogadro software; metal organic framework (MOF); optimization energy; molecular weight; computational simulation; force field; organic carbon links

Citation: Rajendran, P.; Rathinasabapathy, R.; Chandra Kishore, S.; Bellucci, S. Computational-Simulation-Based Behavioral Analysis of Chemical Compounds. *J. Compos. Sci.* **2023**, *7*, 196. https://doi.org/10.3390/jcs7050196

Academic Editors: Thanasis Triantafillou and Francesco Tornabene

Received: 1 March 2023
Revised: 13 April 2023
Accepted: 1 May 2023
Published: 10 May 2023

1. Introduction

In general, behavioral analysis is the study of behavior with respect to the composition and structure of substances. In addition to studying structures, interactions between molecules also play a major role in acquiring the stability of the chemical compound. In this work, stability is examined based on the analysis of two important measures, the optimization energy and molecular weight of various compounds. Molecular weight is the unit of measurement used to describe a molecule's mass. Every molecule has a unique atomic weight that corresponds to the average of its atomic masses. Combining the atomic weights of each atom in a molecule gives the molecular weight. It is a crucial tool for obtaining the ideal operating conditions and required design parameters, and is used for formulating all the material composite model structures with energy minimization [1]. The computational part was carried out with the help of Avogadro software. Avogadro software is used to determine the optimization energy; it is necessary to use the auto-optimization energy tool since it allows users to assign inputs for a variety of compounds as well to view the output files. Before optimization, the lengths and angles of the links and joints do not persist in the exact geometry. During the optimization, the lengths and angles of the links and joints are secured with appropriate geometry and convey optimized

energy. Thus, variation in the angles and bond lengths of organic links and joints within the structured formation of different chemical compounds specifies the optimized energy. These optimized chemicals have a vital role in making metal organic frameworks for supercapacitors. In recent times, chemical compounds that provide high stability have been used to enhance the quality of life in battery-based electronic appliances. Through this analysis, if high-stability chemical compounds are modeled, these can be used as coatings on MOF layers to enhance the quality of appliances.

Previous research mimicked the nanofluid flowing inside the Al nanochannel, which is made up of Al nanoparticles dispersed in Al as the base fluid. For the atomic structure of nanofluids, profiles of physical characteristics such as potential energy, density, velocity, and temperature are computed. These calculations demonstrate that the vacancy defect leads to a decrease in density and an increase in velocity [2]. The binding modes of the molecules with the lowest docking score values were used for subsequent molecular dynamics (MD) simulations in conjunction with free-energy calculations because the experimental crystal structures in a complex with hGSTP1-1 have not yet been established. The Q5 software package was applied to perform Assisted Model Building with Energy Refinement (AMBER) and measure GAFF force fields, and calculate the free energy of several molecules [3]. To increase efficiency and reduce the systems' size in thermal conductivity (Knf) of water–copper, NF was examined as a function of nanochannel wall temperature, copper nanoparticle (NP) size, and force field type (DREIDING, Universal Force Field (UFF), and CHARM) [4]. In recent work, Avogadro software has been used for simulating the interaction between 12 metal atoms with an apigenin model structure to determine the energy minimization. This research was crucial for overcoming the problem of drugs adhering to nanoparticles. To improve the stability, one metal atom was added to the structure of apigenin, for which zinc was formulated as the most suitable metal atom [4].

Among the existing techniques, computational modeling of structures is mainly used to assist the chemicals to form a structure and also to calculate the parameters involved in the structures [5]. In the current situation, many software packages are used for modeling the structure based on the computational process. An advanced molecular editor and visualizer have been created for cross-platform use. Avogadro is a project for computational chemistry, molecular modeling, materials science, and related subjects [6]. Another important parameter considered was optimization energy, which is the means of finding the arrangement of chemical compounds according to a computational model of chemical bonding. In this research, these two important measures were obtained using Avogadro software, which is a progressive molecular editor and visualizer designed for cross-platform use in simulating the chemical models [7]. It includes a strong plugin architecture, flexibility, and high-quality rendering, and common uses include construction of molecular structures, setting up input files, and examining the results of numerous computational chemistry software programs. The purpose of Avogadro is to improve the semantic accessibility of chemical data types by utilizing the Chemical Markup Language (CML) file format [8]. Even in Indium-silico investigation, a metal-nanocomposite structure with the antiviral medicine ribavirin using 12 metals was devised using Avogadro software. This structure was then subjected to energy minimization [9]. Additionally, research facilities have examined a growing number of metal-based medications for their antiviral activity using Avogadro software. In theoretical research on previously published biologically active complex compounds of vanadium, for molecule structural clarification and optimization, DFT calculation investigations have been carried out [10]. The force field of the diverse MMFF94 in the Avogadro program can be used to perform the structural and electronic characterization of the drug. Through the semi-empirical approach, these calculations are carried out to determine the particle's fundamental attributes, which are known to be its stable energy conformation, potential energy, and formation heat. The optimized energy was obtained by linear optimization through traditional force field calculations using the Avogadro setup of the MMFF94 diverse steepest descent until reaching the point

of the lowest degree of potential energy and the empirically more stable conformation of its endemic form [11].

Avogadro is an editor and visualizer for molecules. It is also a piece of software used in science. Avogadro is particularly helpful in the classroom because it aids in the creation of accurate models. In recent research, keto and enol forms of the molecule were created using the Avogadro 1.1 software in consideration of the compound's biological significance. The performance of each compound can be determined based on its properties. This software also allows the determination of the properties, such as molecular and atomic bonds of both forms of the compound, as well as the presence of a response between them [12]. A study developed using Avogadro software investigated the effects of three-dimensional simulations and molecular representations on student conceptual knowledge of chemistry and attitudes toward learning science [13]. There are a large number of parameters used to conduct the structure modeling in Avogadro software. For a better understanding of bio-availability and computational chemistry, analysis of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) analysis, electrostatic potential maps, virtual Fourier transform infrared (FTIR) spectra, statistical thermodynamics parameters, and chemo-metrics was undertaken [14].

An ongoing international scientific effort to precisely determine parameters has produced new findings by isotopically investigating the atoms to improve silicon crystal. The Avogadro constant can be obtained and used to calculate other newly improved parameter measurements [15].

Both specialists and learners will find it easy to perform calculations and visualize the results owing to the band structure and graphical user interface. Fast simulations of the electrical structures of 1D, 2D, or 3D periodic chemical compounds are made possible by Avogadro [16]. The conversion from 2D to 3D structures was performed using Avogadro software. PDF files of HSA and TFE were generated using Avogadro software [17,18]. In this research, UFF, GAFF, and Ghemical Force Field are considered for analysis [19,20]. UFF generally reproduces the most structural features across the periodic table with parameters such as bond lengths and bond angles for almost all elements [21,22]. All structures were plotted with Avogadro software [23,24]. Ghemical is mainly used for molecular dynamics and energy optimization; in addition, it executes geometries of organic carbon links in compounds [25,26]. The performance of GAFF in optimization is encouraging [27]. MOFs are crystalline substances made up of stiff organic molecules that are ordered and kept together by metal ions or clusters [28]. All these quantitative terms have been parameterized and are collectively referred to as the 'forcefield' [29,30]. The energy surface's characteristics are frequently taken into account while determining the step's size [31]. Each element occupies a site of lower potential energy within the structure and makes the overall potential energy of the structure as small as possible; thus, the energy is reduced during the optimization [32]. For a straight or flat surface, larger steps would be more effective than for a slender or narrow modified valley, when more steps of a smaller size would be more appropriate [33]. UFF optimizes well with inorganic materials and organic materials [34]. The geometry optimization procedure calculates the energy at an initial geometry of a molecule and then proceeds to search for a new geometry with a lower energy [35].

Different force fields have been applied in the existing work. Among these force fields, we utilize only three force fields. In this research, widely considered chemical compounds in MOF layers, such as Aluminum, Boron, Calcium, Chlorine, Potassium, Scandium, Tungsten, Indium, and Silicon, were considered for computation and analysis. The use of the UFF force field through the Avogadro software results in the lowest energy consumed by the compounds so that energy minimization occurs. The chemical compounds are attached in the structure to carbon and oxygen. With the energy minimization process, the angle length and bond length are reduced from the structure. In recent work, due to their poor solubility and bio-availability, drugs in BCS Classes II and IV pose a significant challenge to formulators. The BCS IV molecule alectinib hydrochloride (ALB) has very poor solubility, which results in low bio-availability. The goal is to use the Amorphous Solid

Dispersion (ASD) method to increase the solubility and dissolution of ALB using Avogadro software using the Universal Force Field (UFF) with the steepest descent algorithm. The energy-minimized structures are then fed to Autodock4 software [36]. In the existing process, interaction between the aspirin and protein's atomic behavior in the water system is encased in a metallic nanochannel at the same moment. The Cu nanochannel conditions were in a balanced state, and the molecular dynamics (MD) method was applied to achieve this objective. Atomic architecture also made use of Avogadro. There is also the belief that UFFs serve important interatomic purposes [37]. The compounds were analyzed for energy minimization using the Avogadro 1.2.0 software prior to molecular docking. UFF in the Avogadro software optimized the compounds' molecular geometries and employed the steepest descent method to minimize their structural complexity [38,39]

2. Materials and Methods

The purpose of this work is to determine the molecular weight and the optimized energy of different compounds using a computational method through the chemical program. The molecular structure of chemical compounds with organic carbon linkers was designed using Avogadro-1.2.0n-win32 for Windows and subjected to energy minimization. Avogadro allows the users to obtain the molecular weight and design practically any compound with the optimized geometry corresponding to different force field options. GAFF is specifically parameterized for organic carbon link compounds made up of C, N, O, H, S, P, F, Cl, Br, and I. In this work, energy minimization of chemical compounds in all of the three force fields was achieved with a one-dimensional structure. In the one-dimensional structure, the link should be connected firmly; otherwise, during optimization, it will be separated from the structure, and later provide erroneous energy values.

In this research, the general structure considered to join the chemical element and organic carbon links is $M_4O(CO_2)_6$, as this type of structure has been considered for increasing the MOF surface area. Here, M is the material under test and is changed for the development of other models. The remaining structure of the formula indicates the organic carbon links and oxygen, which remains the same throughout the process. According to this structure, four chemical elements are joined with a single oxygen molecule at the center, and then six carbon dioxide molecules are connected around the chemical compounds. The entire elements should be linked with each other. For developing other models, only M has to be changed, namely, Al, Br, Ca, Cl, In, K, Sc, Si, and W. In total, nine elements were considered for analysis. The selected elements were made up of the combination of metal and nonmetal in order to study the behavior of both. In this research, the choice of elements was considered from a total of nine: four were metals, four were nonmetals, and the remaining one was metalloid.

2.1. Molecular-Weight-Based Analysis

Molecular weight is a very important parameter for the design of structured chemical compounds. The unit of molecular weight is g/mol and the molecular weight increases with the mechanical characteristics of the material. However, the mechanical property is typically unaffected over a certain limiting value of the molecular weight. Therefore, the stability is also associated with molecular weight. The firmness of the molecular structure depends on the physical, chemical, and mechanical properties, such as mechanical strength, resistance, viscosity, and melting point. In this research, the molecular weight of different chemical compounds was calculated using the computational method within Avogadro software. To determine the molecular weight, the formulated structure $M_4O(CO_2)_6$ is initially framed for different chemical compounds, and the molecular weight is then calculated using a property tool. In general, molecular weight is calculated before starting the energy reduction as the molecular weight does not change while optimizing energy and remains constant in all three force fields. The molecular weight of various chemical compounds with organic carbon links configured using Avogadro software before applying any force field is shown in Figure 1, and the same is tabulated in Table 1. From Table 1, it is

observed that the molecular weight of tungsten remains high, with the value of 1027.512 g mol^{-1}, whereas boron has the least molecular weight, of 335.396 g mol^{-1}.

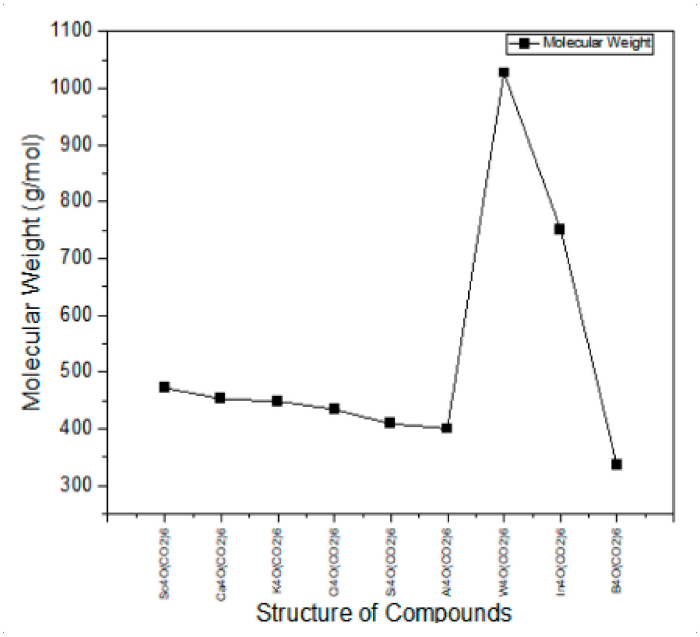


Figure 1. Molecular weight of different compounds.

Table 1. Molecular weight of compounds under testing.

Name of the Element	Structure of Compounds	Molecular Weight g mol^{-1}
Scandium	$Sc_4O(CO_2)_6$	471.975
Calcium	$Ca_4O(CO_2)_6$	452.464
Potassium	$K_4O(CO_2)_6$	448.545
Chlorine	$Cl_4O(CO_2)_6$	433.964
Silicon	$Si_4O(CO_2)_6$	408.525
Aluminum	$Al_4O(CO_2)_6$	400.078
Tungsten	$W_4O(CO_2)_6$	1027.512
Indium	$In_4O(CO_2)_6$	751.424
Boron	$B_4O(CO_2)_6$	335.396

2.2. Energy Minimization

When arranging chemical elements in space, energy minimization is crucial since certain chemical structures may not be advantageous from an energetic approach [30]. Energy minimization may also be known as energy reduction or energy optimization. Finding a set of coordinates that represent the minimum energy conformation for the given structure is the aim of energy reduction. When correcting structural anomalies, energy minimization is a crucial tool for locating the closest local minima [30]. Avogadro finds the most stable form and the lowest energy of the molecule by minimizing all the interactions within the molecule using advanced algorithms and applying a force field.

The optimized energy of the chemical elements in molecular mechanics is calculated using the force field concept. One of the most crucial representative parameters of a molecule's stability is its energy in a force field. In general, the force field is used to minimize the bond stretching and angle length. In this research, energy minimization is carried out through the auto-optimize tool in Avogadro software. This tool furnishes an

interactive interface among the elements in the structure, allowing it to handle elements while its molecular geometry is being optimized.

The auto-optimization settings provide several force fields options; among these, only three force fields were selected for this work, since these are applicable to non-periodic property structure modeling where atomic mass increases without variation in the structure. By clicking the auto-optimization tool, the structure built using the Avogadro software will be optimized by making changes in the bond length and its angle. Thus, while optimization occurs, the size of the compound structure is reduced. Each element occupies a site of lower potential energy within the structure, making the overall potential energy of the structure as small as possible; thus, the energy is reduced during the optimization [32]. Finally, the optimized energy value is calculated and displayed at the top-right corner of the screen. This generates a structure with greater stability, and as the optimization energy decreases, the stability of the compounds increases. At first, the structure of the compounds is modeled as shown in Figure 2, which is a before-optimization structure. The same structure of chemical compounds with an organic carbon link and joints was adapted for all the force fields. Next, an individual force field is applied to each compound; subsequently, energy reduction by means of the steepest decent algorithm is carried out, and then optimized energy is evaluated. The optimized structures of various chemical compounds with their organic carbon links and joints under various force fields are shown in Figure 3.

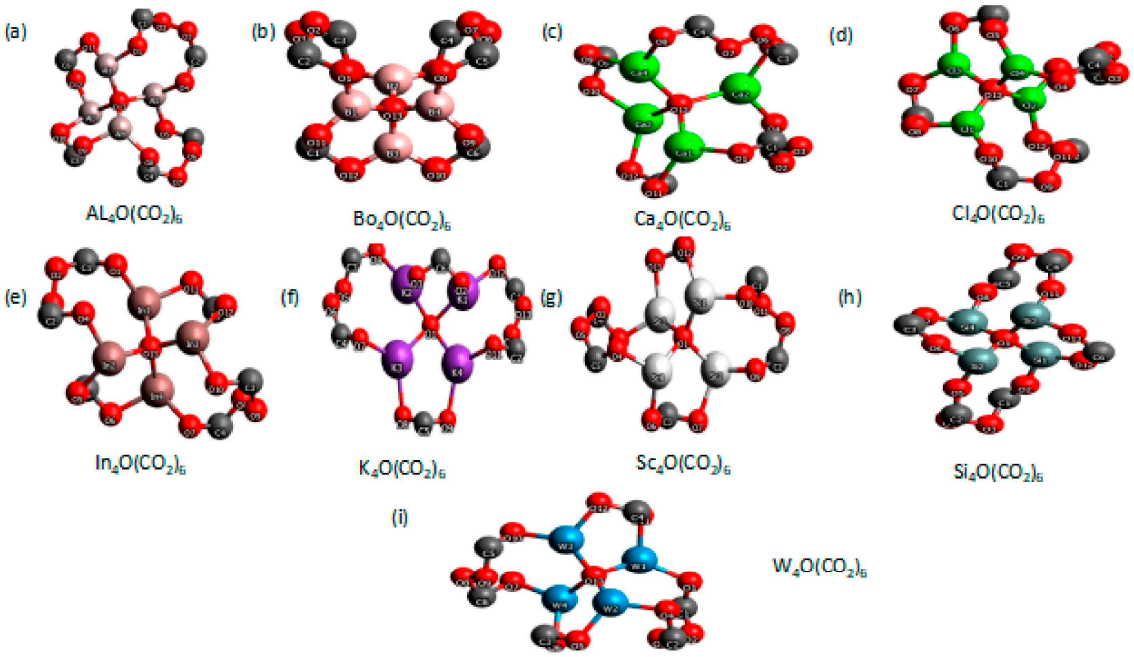


Figure 2. Structure of compounds before the energy optimization.

Here, UFF, GAFF, and Ghemical force fields are used with parameters to create molecular structures with optimization. Molecular structures considered for different compounds were optimized under these force fields. The energy values of each material differ based on the applied force field. In Avogadro software, the default algorithm for energy reduction is the steepest descent algorithm. The storage and computing needs are just two of the factors that affect the choice of minimization strategy. Whenever the initial structure is far from the minimum, conjugate gradients may not be as effective as the steepest descent approach. However, after the initial tension is eliminated, conjugate gradients perform far better. Since molecular mechanics is always used in system calculations, the steepest descents and conjugate gradients techniques are often used in this context. The step size at the beginning of the steepest descents algorithm, which is used in the majority of molecular modeling applications, has a fixed default value. After the initial iteration, if energy drops,

the step size is increased for the subsequent iteration through an increasing component. The process continues until the energy level decreases with each iteration. It is presumed that the algorithm has jumped across the valley that makes up the lowest level and up the incline on the opposite face when a step results in an increase in energy. A multiplicative factor is then used to lower the step size (e.g., 0.5).

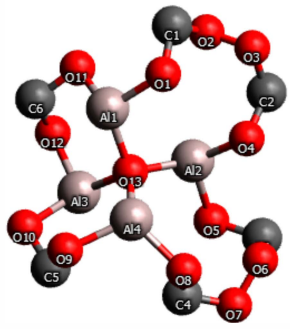
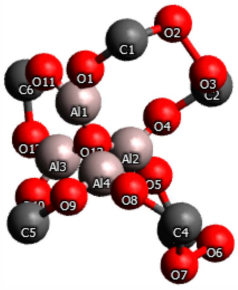
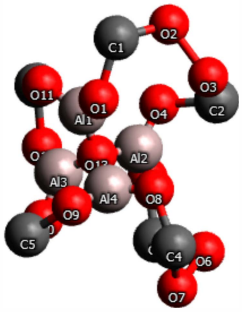
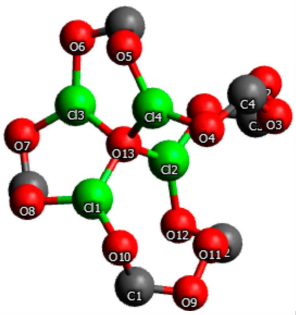
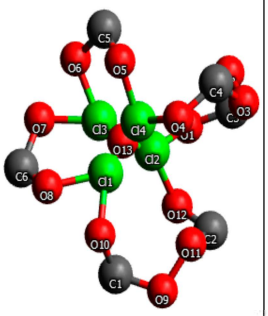
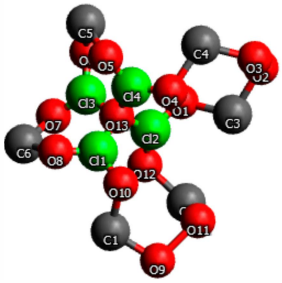
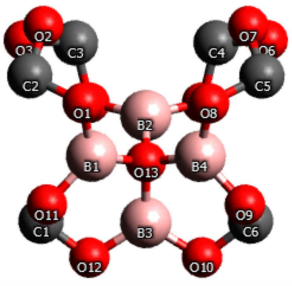
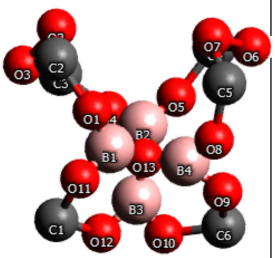
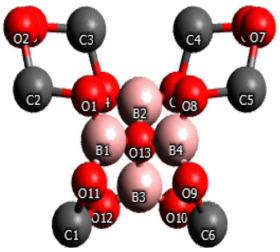
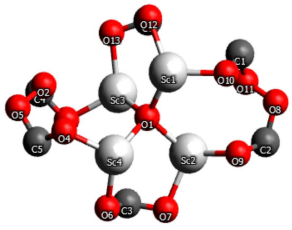
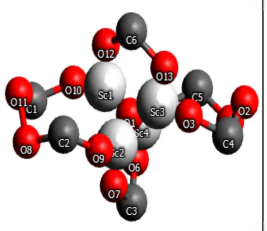
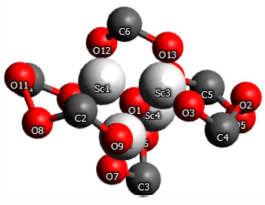
Force Field/Elements	**(a) UFF**	**(b) GAFF**	**(c) Ghemical**
Aluminum			
Chlorine			
Boron			
Scandium			

Figure 3. *Cont.*

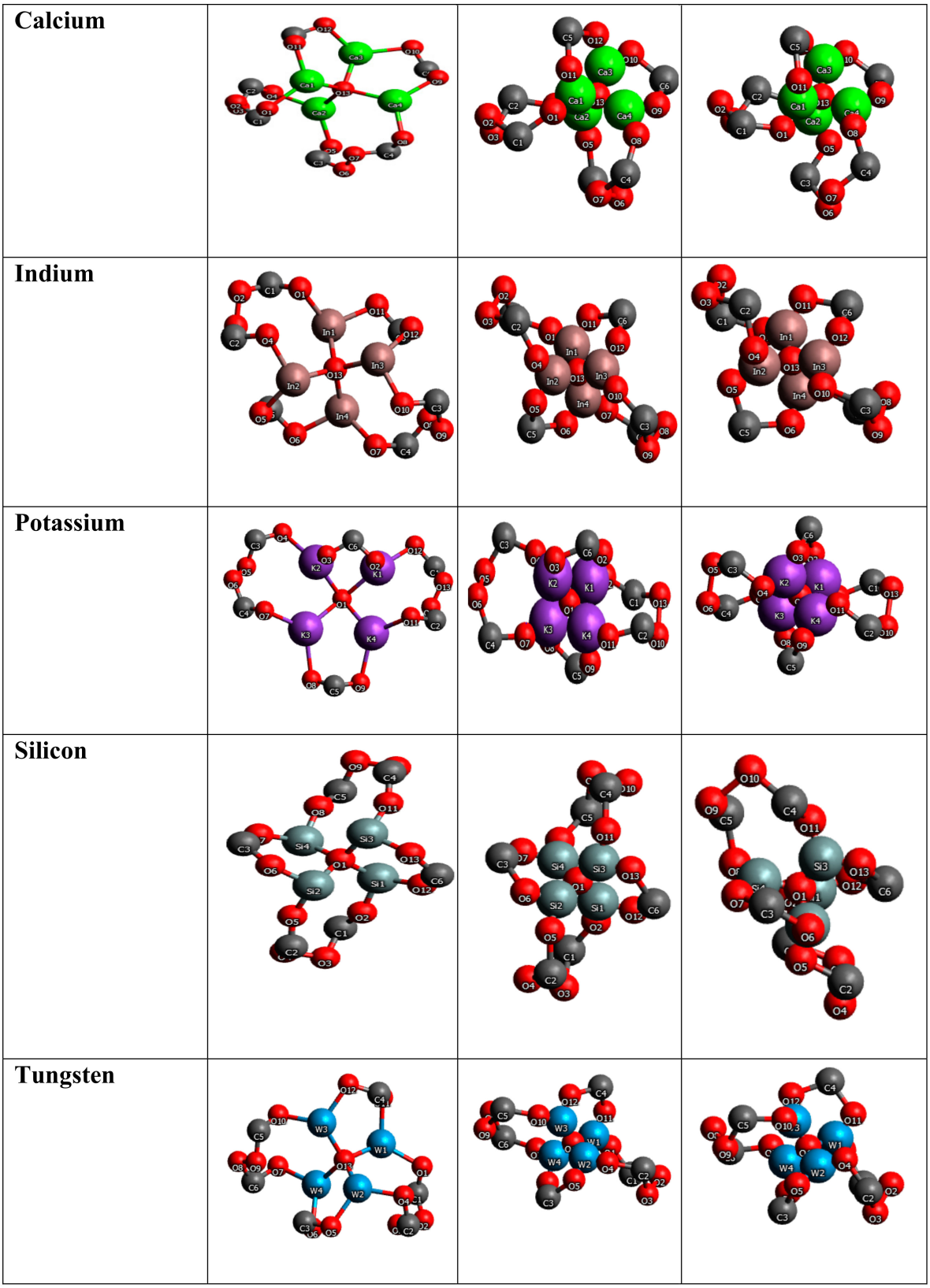


Figure 3. Optimized structure of examined compounds with organic carbon links using (**a**) UFF, (**b**) GAFF, and (**c**) Ghemical force field.

Figure 3 represents the optimized energy structure of various compounds under UFF, GAFF, and Ghemical force fields. The values of optimized energy of different compounds

under the three force fields are shown in Table 2. Comparing the results of energy reduction obtained under different force fields, each provides low energy for different chemical compounds organized in the form of a graph based on the optimized value shown in Figure 4. In this research, under UFF, the lowest energy of 22.673 kJ mol^{-1} was delivered by the In-based compound; under GAFF, the lowest energy of 3.650 kJ mol^{-1} was delivered by the Si-based compound; and under the Ghemical force field, the lowest energy of 136.234 kJ mol^{-1} was delivered by the K-based compound. The energy details of these three top compounds under different force fields are tabulated separately in Table 3 and also indicated in the corresponding graph in Figure 5.

Table 2. Optimized energy of compounds under various force fields.

Compounds under Test	Optimized Energy (kJ mol^{-1})		
	UFF	GAFF	Ghemical
$Al_4O(CO_2)_6$	84.0046	651.771	153.093
$Cl_4O(CO_2)_6$	2394.62	69.102	340.094
$B_4O(CO_2)_6$	233.334	37.88	161.813
$Sc_4O(CO_2)_6$	57.358	33.655	156.806
$Ca_4O(CO_2)_6$	204.573	36.916	165.211
$In_4O(CO_2)_6$	22.673	35.396	150.126
$K_4O(CO_2)_6$	890.684	33.694	136.234
$Si_4O(CO_2)_6$	1717.15	33.654	156.806
$Al_4O(CO_2)_6$	244.688	35.396	150.126

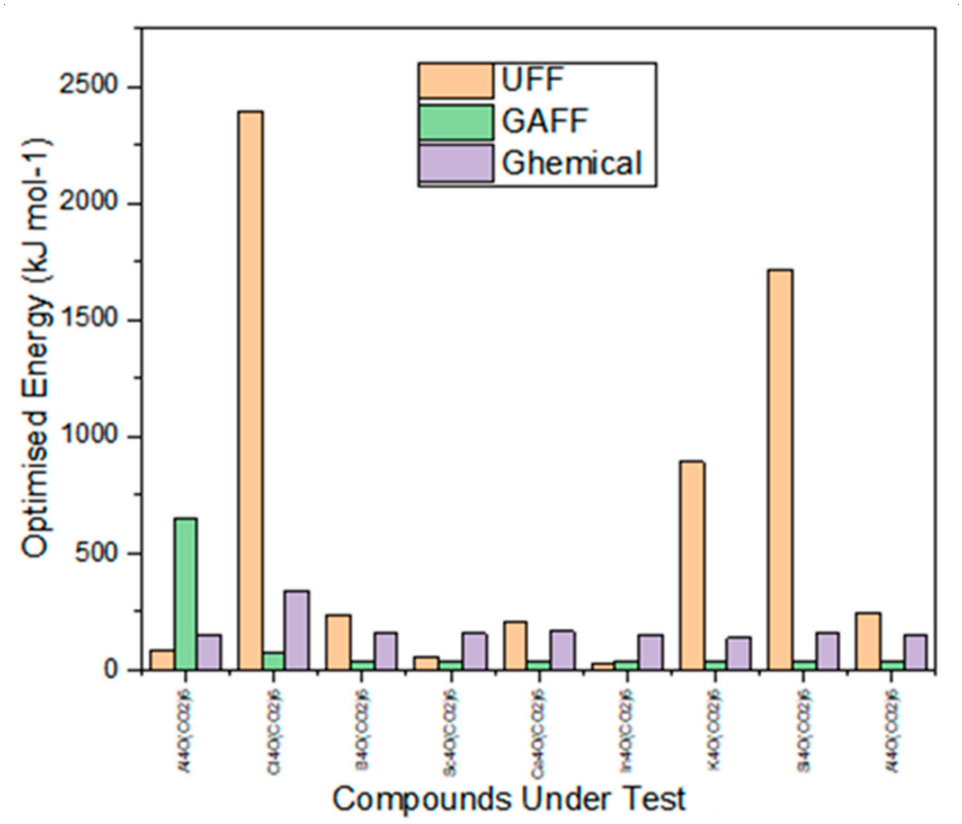


Figure 4. Optimized energy of compounds in three force fields.

Table 3. Optimized energy of top compounds in force fields.

	Optimized Energy (kJ mol^{-1})		
Force Fields/Top Compounds	**UFF**	**GAFF**	**Ghemical**
$In_4O(CO_2)_6$	22.673	57.358	890.684
$Sc_4O(CO_2)_6$	35.3955	33.655	33.694
$Si_4O(CO_2)_6$	150.126	156.806	136.234

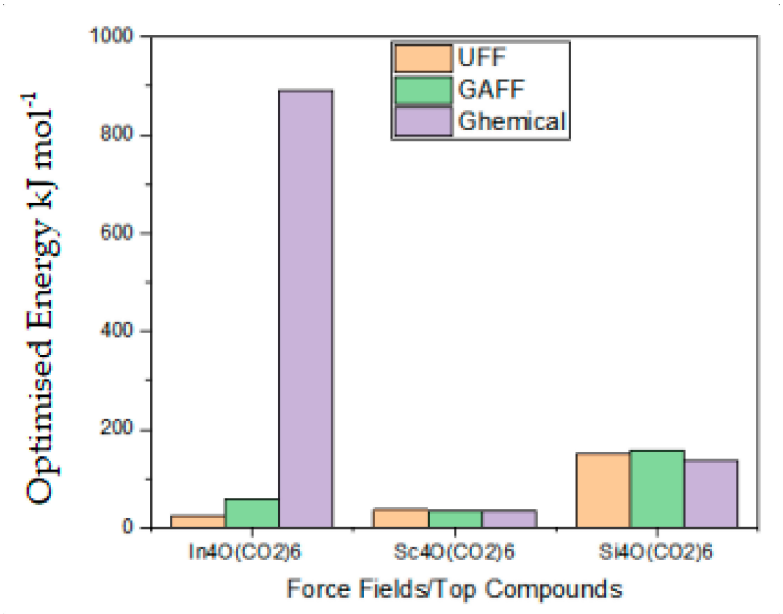


Figure 5. Comparison of top compounds with optimized energy in three force fields.

From the above study, we conclude that the present research work mainly concentrated on the chemical compounds that react with the organic linker and produce less energy. The lower energy value obtained will be considered as the best chemical compound for the MOF framework. With the help of the optimization, the structure is optimized through different force fields. Among these three force fields, UFF shows less energy when compared, and it is able to finalize the chemical compound for the MOF framework. In future, this work can be extended for determining the schemes of material properties of other chemicals with similar processes using Avogadro software. The work can be extended by adding more chemical compounds which can be tested. This work can also be implemented using different organic carbon linkers, and can be used to analyze the bond and angle length of different chemical compounds.

In previous research work, Zr showed the lowest optimized energy of 320 kJ/mol [40]. The present research showed that Indium has the lowest optimized energy when compared with the optimized shapes of the metals with a joint complex, i.e., Zr-based (320 kJ/mol^{-1}) [40]. A comparison between two compounds with energy optimized in the force fields is shown in Figure 6. In this research, we added a few chemical compounds to enhance the amount of storage capacity. Through this work, we aimed to discover whether MOF particles are replaceable as dielectrics for supercapacitors and to determine the efficiency. The In-based joint showed 22.673 kJ mol^{-1} in UFF. We simultaneously investigated the MOF molecules' functionality and stability, and this study was able to identify better chemical compounds that required less energy for optimization. It takes more work to stabilize the complex since the greater the functionality, the more heat (enthalpy) it can emit. We want complexity to be more stable and efficient, as well as more porous. The trade-off between utility and stability is constant.

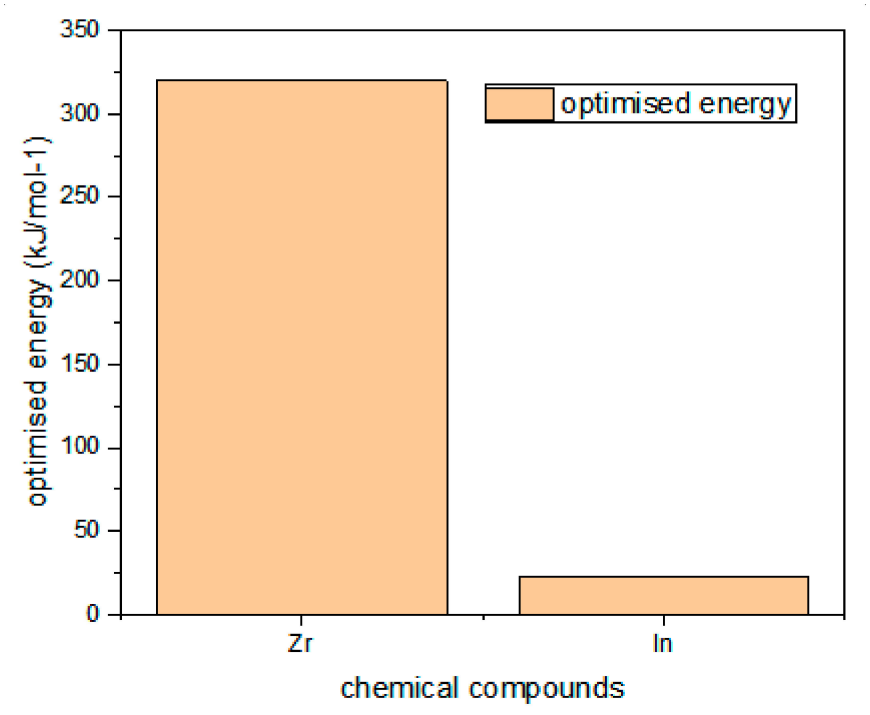


Figure 6. Comparison between two compounds with optimized energy in force fields.

3. Conclusions

This research examines the grade of materials with respect to energy reduction in three different force fields. That is, the stability of compounds is analyzed in the force fields with respect to energy minimization. If the energy decreases, the stability of material increases; thus, the grade also increases. Practically, because there is more energy (enthalpy), more can be provided, meaning that it requires more effort to stabilize the chemical compound. The molecular modeling, geometry optimization, and characterization of considered compounds were performed and investigated. Optimization of molecular-independent energy on a computational graph is proposed and demonstrated in this work by carrying out geometry optimization. Geometrical parameters such as bond lengths and bond angles and dihedral angles of different compounds were optimized to find the best atomic arrangement that makes the molecule more stable. Molecular structure and energy reduction in various force fields of different chemical compounds were established using Avogadro software. The optimization energy was simulated by varying the geometry of organic carbon links and the results were shown. The top chemical compounds with the lowest energy in three different force fields were the In-based joint, with 22.673 kJ mol^{-1} in UFF; the Si-based joint, with 33.650 kJ mol^{-1} in GFF; and the K-based joint, with 136.234 kJ mol^{-1} in Ghemical force field. Comparison results show that among the top compounds from each force field, the In structure has greater energy reduction of 22.673 kJ mol^{-1} in UFF when compared with the other two force fields. We could design an effective optimization protocol from this research. The impact of choosing a proper force field for optimization is discussed in this work and investigations show that UFF is suitable for optimizing the most compounds, and hence serves as the optimal choice for energy reduction. However, confusingly, the analyzed structure obtained both local minima and global minima. The molecular weights of the chemical compounds obtained using Avogadro were also analyzed. The molecular weight of W remains high, at 1027.512 kJ mol^{-1}, whereas B has the least molecular weight, of 335.396 kJ mol^{-1}. From the results, it was concluded that higher-molecular-weight compounds are more stable than lower-molecular-weight compounds, except W, because the combination of W with carbon will easily break the chain or bond between them. Thus, even when the molecular weight is high for W, it does not have stability. The short-term strength of W has a propensity to decrease when carbon is added, because W has a low

melting point and the bond strength also does not decrease when the optimization is carried out. Thus, a high molecular weight improves the stability of all types of considered chemical compounds due to molecular interactions.

Author Contributions: Conceptualization, P.R.; methodology, R.R., S.C.K. and P.R.; software, P.R.; validation, R.R. and P.R.; formal analysis, P.R. and R.R.; investigation, R.R., S.B., S.C.K. and P.R.; resources, R.R. and P.R.; data curation, P.R.; writing—original draft preparation, P.R.; writing—review and editing, R.R., S.C.K. and P.R.; supervision, R.R., S.C.K. and S.B.; project administration, P.R. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: All data are available in the article.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Nath, A.; Hazra, D.; Pal, R. Formulation of nano-composite model structures using apigenin with several materials using in silico approach. *Int. J. Biotechnol. Microbiol.* **2021**, *3*, 42–45.
2. Alazwari, M.A.; Abu-Hamdeh, N.H.; Nusier, O.K.; Karimipour, A. Vacancy defect influence on nanofluid flow and absorbed thermal energy in a nanochannel affected by Universal Force Field via composed approach of embedded atom model/molecular dynamics method. *J. Mol. Liq.* **2021**, *333*, 115927. [CrossRef]
3. Pantiora, P.; Furlan, V.; Matiadis, D.; Mavroidi, B.; Perperopoulou, F.; Papageorgiou, A.C.; Sagnou, M.; Bren, U.; Pelecanou, M.; Labrou, N.E. Monocarbonyl Curcumin Analogues as Potent Inhibitors against Human Glutathione Transferase P1-1. *Antioxidants* **2023**, *12*, 63. [CrossRef] [PubMed]
4. Yu, Q.; Alameri, A.A.; Alizadeh, A.; Hekmatifar, M.; Al-Khafaji, M.O.; Shabolaghi, K.R.; Ahmad, N.; Alshehri, A.; Nassajpour-Esfahani, N.; Toghraie, D.; et al. Molecular dynamics simulation of thermal behavior of nanofluid flow in a nanochannel with Cetryltrimethylammoniu Bromide surfactant molecules. *J. Mol. Liq.* **2023**, *369*, 120938. [CrossRef]
5. Snyder, H.D.; Kucukkal, T.G. Computational chemistry activities with Avogadro and ORCA. *J. Chem. Educ.* **2021**, *98*, 1335–1341. [CrossRef]
6. Hanwell, M.D.; Curtis, D.E.; Lonie, D.C.; Vandermeersch, T.; Zurek, E.; Hutchison, G.R. Avogadro: An advanced semantic chemical editor, visualization, and analysis platform. *J. Cheminformatics* **2012**, *4*, 1–17. [CrossRef] [PubMed]
7. Arghya, N.; Singh, D.; Mukherjee, N. Ribavirin-Material Nanocomposite Structure Developed through Computational Approach: Formulation of Antiviral Drug by In Silico Method. 2022. Available online: https://www.researchgate.net/profile/Arghya-Nath/publication/360748317_Ribavirin-Metal_Nanocomposite_Structure_Developed_Through_Computational_Approach_Formulation_Of_Antiviral_Drug_By_In_Silico_Method/links/6287d6ae39fa217031608446/Ribavirin-Metal-Nanocomposite-Structure-Developed-Through-Computational-Approach-Formulation-Of-Antiviral-Drug-By-In-Silico-Method.pdf (accessed on 28 February 2023).
8. Vlasiou, M.C.; Pafti, K.S. Screening possible drug compound s for COVID-19. The example of vanadium (III/IV/V) complex compound s with computational chemistry and molecular docking. *Comput. Toxicol.* **2021**, *18*, 100157. [CrossRef]
9. Lokhande, K.B.; Nagar, S.; Swamy, K.V. Molecular interaction studies of Deguelin and its derivatives with Cyclin D1 and Cyclin E in cancer cell signaling pathway: The computational approach. *Sci. Rep.* **2019**, *9*, 1–13. [CrossRef]
10. Miqueias, R.; Marinho, M.M.; Marinho, E.S. Structural Characterization of the Hypoglycemic Drug Glimepiride. *Int. J. Recent Res. Rev.* **2018**, *11*, 26–35.
11. Katanguru, L. Characterization of Keto and Enol forms of Indoline-2, 3-Dione-3-Oxime using Avogadro Software Tool–A Theoretical Study. *Orient. J. Chem.* **2018**, *34*, 1270.
12. Azuma, Y.; Barat, P.; Bartl, G.; Bettin, H.; Borys, M.; Busch, I.; Cibik, L.; D'agostino, G.; Fujii, K.; Fujimoto, H.; et al. Improved measurement results for the Avogadro constant using a 28Si-enriched crystal. *Metrologia* **2015**, *52*, 360. [CrossRef]
13. Zia, M.K.; Siddiqui, T.; Ali, S.S.; Ahsan, H.; Khan, F.H. Exploring the interaction of anti-androgen drug-bicalutamide with human alpha-2-macroglobulin: A biophysical investigation. *Int. J. Biol. Macromol.* **2018**, *120*, 2285–2292. [CrossRef]
14. Naeem, A.; Iram, A.; Bhat, S.A. Anesthetic 2, 2, 2-trifluoroethanol induces amyloidogenesis and cytotoxicity in human serum albumin. *Int. J. Biol. Macromol.* **2015**, *79*, 726–735. [CrossRef]
15. Karimian, N.; Gholivand, M.; Taherkhani, F. Computational design and development of a novel voltammetric sensor for minoxidil detection based on electropolymerized molecularly imprinted polymer. *J. Electroanal. Chem.* **2015**, *740*, 45–52. [CrossRef]
16. Husain, M.A.; Ishqi, H.M.; Sarwar, T.; Rehman, S.U.; Tabish, M. Interaction of indomethacin with calf thymus DNA: A multi-spectroscopic, thermodynamic and molecular modeling approach. *MedChemComm* **2017**, *8*, 1283–1296. [CrossRef] [PubMed]
17. Tahir, M.N.; Khalid, M.; Islam, A.; Mashhadi, S.M.A.; Braga, A.A. Facile synthesis, single crystal analysis, and computational studies of sulfanilamide derivatives. *J. Mol. Struct.* **2017**, *1127*, 766–776. [CrossRef]
18. Jaillet, L.; Artemova, S.; Redon, S. IM-UFF: Extending the universal force field for interactive molecular modeling. *J. Mol. Graph. Model.* **2017**, *77*, 350–362. [CrossRef]

19. Rappe, A.K.; Casewit, C.J.; Colwell, K.S.; Goddard, W.A.; Skiff, W.M. UFF, a full periodic table force field for molecular mechanics and molecular dynamics simulations. *J. Am. Chem. Soc.* **1992**, *114*, 10024–10035. [CrossRef]
20. Toby, L.-A.; Townsend, P.A.; Grayson, M.N. Comparisons of different force fields in conformational analysis and searching of organic carbon links compound s: A review. *Tetrahedron* **2021**, *79*, 131865.
21. Ádám, J.; Rák, Á.; Ladjánszki, I.; Cserey, G. Optimized GPU implementation of merck molecular force field and universal force field. *J. Mol. Struct.* **2019**, *1188*, 227–233.
22. Ricardo, G.; Gobato, M.R.R.; Heidari, A. Calculation by UFF method of frequencies and vibrational temperatures of the unit cell of the rhodochrosite crystal. *Int. J. Adv. Chem.* **2019**, *7*, 77–81.
23. Sprenger, K.G.; Jaeger, V.W.; Pfaendtner, J. The general AMBER force field (GAFF) can accurately predict thermodynamic and transport properties of many ionic liquids. *J. Phys. Chem. B* **2015**, *119*, 5882–5895. [CrossRef] [PubMed]
24. Junmei, W.; Wolf, R.M.; Caldwell, J.W.; Kollman, P.A.; Case, D.A. Development and testing of a general amber force field. *J. Comput. Chem.* **2004**, *25*, 1157–1174.
25. Altınbaş, Ö.G.; Peukert, W.; Clark, T. An improved generalized AMBER force field (GAFF) for urea. *J. Mol. Model.* **2010**, *16*, 1427–1440.
26. Padmaja, W.; Velayutham, R.; Roy, K.K. Structure investigation, enrichment analysis and structure-based repurposing of FDA-approved drugs as inhibitors of BET-BRD4. *J. Biomol. Struct. Dyn.* **2019**, *37*, 3048–3057.
27. Nazanin, D.; Dickson, A. Predicting partition coefficients for the SAMPL7 physical property challenge using the ClassicalGSG method. *J. Comput.-Aided Mol. Des.* **2021**, *35*, 819–830.
28. Lee, V.S.; Chong, W.L.; Sukumaran, S.D.; Nimmanpipug, P.; Letchumanan, V.; Goh, B.H.; Lee, L.H.; Zain, S.M.; Abd Rahman, N. Computational screening and identifying binding interaction of anti-viral and anti-malarial drugs: Toward the potential cure for SARS-CoV-2. *Prog. Drug Dis. Biomed. Sci.* **2020**, *3*. [CrossRef]
29. Amara, J.; Mohamedali, A.; Ranganathan, S. Protocol for protein structure modelling. In *Encyclopedia of Bioinformatics and Computational Biology: ABC of Bioinformatics*; Elsevier: Amsterdam, The Netherlands, 2019; pp. 252–272.
30. Budhayash, G. Energy Minimization. In *Homology Molecular Modeling: Perspectives and Applications*; Maia, R., de Moraes Filho, R., Campos, M., Eds.; IntechOpen: London, UK, 2020. [CrossRef]
31. Shinde, P.A.; Abdelkareem, M.A.; Sayed, E.T.; Elsaid, K.; Olabi, A. *Metal Organic Frameworks (MOFs) in Supercapacitors*; Olabi, A.-G., Ed.; Encyclopedia of Smart Materials Elsevier: Amsterdam, The Netherlands, 2022; pp. 414–423.
32. Available online: https://www.researchgate.net/figure/The-Highest-Occupied-Molecular-Orbital-HOMO-and-Lowest-Unoccupied-Molecular-Orbital_fig1_344422007 (accessed on 28 February 2023).
33. Kunal, R.; Kar, S.; Das, R.N. *Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment*; Academic Press: Cambridge, MA, USA, 2015.
34. Donatella, B.; Jäntschi, L. Comparison of molecular geometry optimization methods based on molecular descriptors. *Mathematics* **2021**, *9*, 2855.
35. Adam, L.; Arłukowicz, P.; Czaplewski, C.; Ołdziej, S.; Pillardy, J.; Scheraga, H.A. A method for optimizing potential-energy functions by a hierarchical design of the potential-energy landscape: Application to the UNRES force field. *Proc. Natl. Acad. Scie. USA* **2002**, *99*, 1937–1942.
36. Kumar, S.S.; Joshi, A.; Singh, R.; Jana, S.; Dubey, K. An investigation into solubility and dissolution improvement of alectinib hydrochloride as a third-generation amorphous solid dispersion. *J. Drug Deliv. Sci. Technol.* **2023**, *81*, 104259.
37. Hoang, L.Q.; Heydaripour, S.; Farhadi, B.; Rashid, R.F.; Mustafa Inc. A molecular dynamics investigation of the atomic structural behavior of the interaction between amyloid beta protein and Aspirin within an aqueous nanodomain. *Eng. Anal. Bound. Elem.* **2023**, *146*, 851–858.
38. Yakubu, S.E.; Abugri, J.; Rashid, I.A.; Osei, F.; Ayariga, J.A. In silico Identification of potential Inhibitors of acyl carrier protein reductase and acetyl CoA Carboxylase of Plasmodium falciparum in Antimalarial Therapy. *Front. Drug Discov.* **2023**, *3*, 1.
39. Hakkı, C.İ.; Liman, R.; İstifli, E.S.; Akyıl, D.; Özkara, A.; Bonciu, E.; Colă, F. Cyto-Genotoxic and Behavioral Effects of Flubendiamide in Allium cepa Root Cells, Drosophila melanogaster and Molecular Docking Studies. *Int. J. Mol. Sci.* **2023**, *24*, 1565.
40. Richard, K.; Baek, W.J.; Choung, J.; Kim, A. Study on the Optoelectronic Behavior of Zr Based MOFs Using Computational Simulations. In Proceedings of the 2019 IEEE 9th Annual Computing and Communication Workshop and Conference (CCWC), IEEE, Las Vegas, NV, USA, 7–9 January 2019; pp. 0630–0633.