International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

Vol. 36 No. 2 January 2023, pp. 136-160

Advanced Computer Graphics Aided Molecular Visualization And Manipulation Softwares: The Hierarchy Of Research Methodologies

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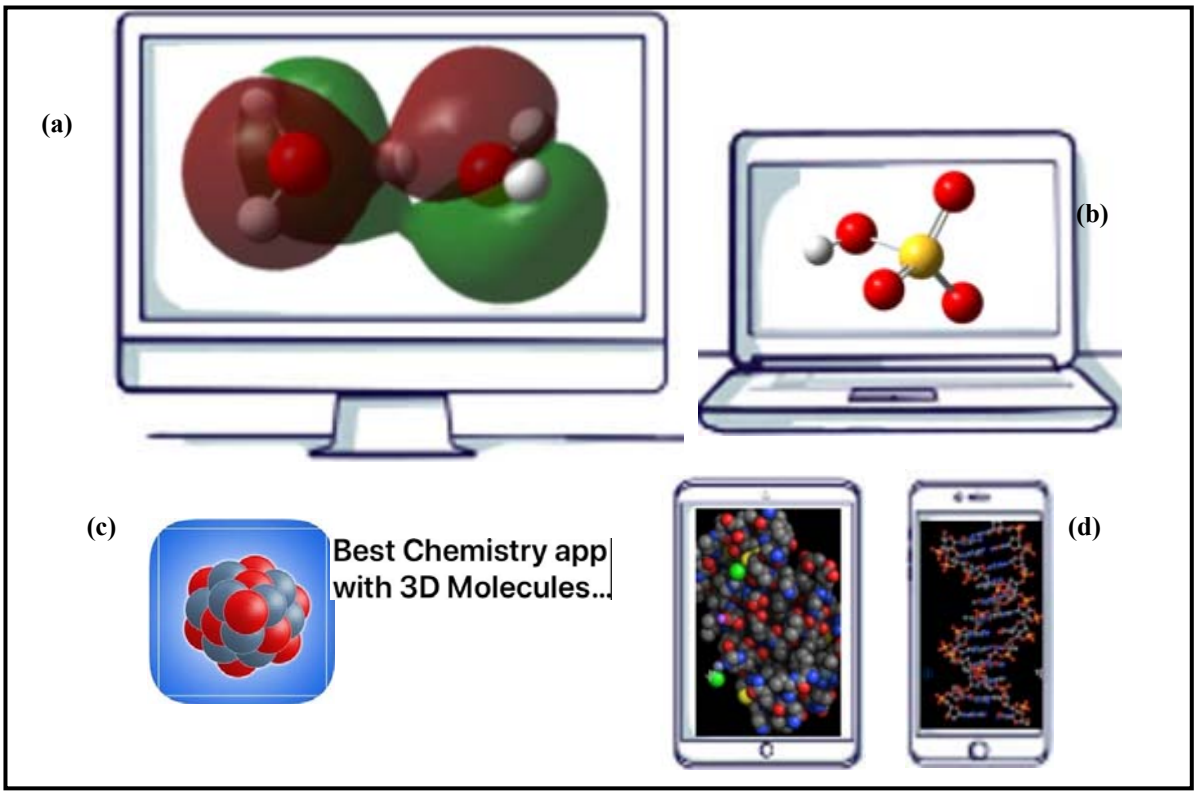
Abstract – In the present day, the huge obstacles, and the major technical problems encountered by the teaching and research faculties, academicians, industrial specialists, laboratory demonstrators and instructors, fellow students and researchers, etc. are to adopt integrative approaches of demonstrating (learning) chemistry and chemical education, and the realistic ways of delivering (grasping) scientific materials articulately with graceful and effortless manner. Towards minimizing these challenges, various audio-visual tools and technologies, advanced computer aided molecular graphics, freely available electronic gadgets assisted chemistry and chemical education apps, human unreadable data reading and accessing softwares, etc. are being incorporated worldwide as the most indispensable physical and electronic means for successful professionalisms. This short article is essentially a collective report underscoring extraordinary approaches, incredible efforts, and innovative skills of the computer based chemical and molecular graphics towards illuminating intrinsic parts of the chemistry and chemical education, and revealing various aspects of the cutting -edge research. As their representatives, herein, the different type computer coding languages based graphical tools such as Molden, GaussView, Jmol, and Visual Molecular Dynamics (VMD) are referred, and elucidated their potential applications and remarkable attempts in the advancement of diverse areas of chemistry and chemical education. Beside this, the most essential graphical features, unique rendering abilities with magnificent views, splendid visualizing skills, awesome data accessing functionalities, etc. of each of them, and their invaluable roles for studying complex molecules, biomolecules, crystals, and the entire material assemblies as well as for investigating global and local molecular physicochemical properties are presented concisely with the special stresses on their relatively better and comparatively more applicable distinctive attributes explicitly

Keywords – Chemistry/Chemical Education, Computer Graphics, Molden, Jmol, GaussView, and Visual Molecular Dynamics (VMD)

I. INTRODUCTION

The literal meaning of the computer graphics is simply the computer based three dimensional sketches, arts, images, drawings, pictorial networks, lines, charts, any types of visuals, and the representations of the data in a graphical manner [1]. With the help of advanced computer programming, mathematical algorithms, 3D modeling Apps, and many other scientific tools, techniques & technologies, all these set of digital images are actually manipulated and created in the form of pixels (the "building blocks" of the digital image), and drawn or displayed on the screen of the magnificent android, iOS or other operating systems supporting electronic gadgets (desktop & laptop computers, iPads, tablets, smartphones, smart television with web browsers, etc.) with preinstalled molecular visualization and manipulation softwares as depicted in Scheme 1 [2]. Shortly reiterating, the computer graphics is a rendering tool that converts binary data codes to real visual images through the basic computational techniques involving computations, manipulations, and digital synthesis of all types of the 3D images [1, 2]. In application point of view, it is widely recognized core technology especially in the field of animated entertainments & amusements, cartography,

digital photography, photo upscaling & enhancement, medical imaging for clinical analysis, climate & weather maps, satellite imaging, engineering drawings, architectures, molecular simulations, molecular modeling, visualization & manipulation of the molecular objects, etc. [1–4]. More particularly, its critical roles and dedications towards the advanced development of chemical science, physical science, biological science, biochemical science, biomolecular science, nanotechnology, medicinal chemistry, drug discovery science, and applied science & engineering since the invention of passive type "Light Pens" devices in 1960s, and active type "Rand Tablet" with OCSS-LHASA (Organic Chemical Synthesis Simulation-Logic and Heuristics Applied to Synthetic Analysis) synthesis planning system & "Acoustic Tablet" in 1970s and Harvard PDP-1 DEC-340 display system & the Princeton PDP-10 E & S LDS-1in 1980s are highly commendable [5]. Since then, its meaningful impact on chemistry and the theory of chemical structure has been recognizing mainly due to its compatibility with various application-dedicated chemistry softwares and Apps related to cheminformatics such as chemical sketchers, manipulators, simulators & visualizers, and their substantial uses for working with chemical & molecular graphics in a user-friendly interface & the remarkable services as a full-set software package equipped with the extraordinary features applicable to the state-of-the-art molecular drawing, editing, publishing, modeling, and analyses [4–8]. As per the *Physics Today*'s special article entitled "Nobel Prize Honors Kohn and Pople for Methods of Quantum Chemistry" [9], the extensive uses & overwhelming acceptance of the chemical and molecular graphics as a quite indispensable tool & technique for the efficient R & D methodologies and the effective chemical education was only after the announcement of 1998 Nobel prize awardee in chemistry (viz., W. Kohn and J. Pople) for their substantial works in computational chemistry and molecular modelling. Accordingly, in the computational drug discovery history, the substantial uses of the chemical graphics was realized only after the successful introduction of the commercial drug-design computational packages targeted to the pharmaceutical industry by Tripos Company in 1979 [8].



Scheme 1. The electronic gadgets with preinstalled visualization & manipulation chemical & molecular graphics softwares displayed molecular models and molecular orbitals of the variably sized chemical compounds. The hand drawn vintage sketch of the gadgets were extracted individually from the image gallery of "*Art of it*", and integrated here. The three dimensional ball-stick models of the giant biomolecules shown on the screen of the smart tablet and smart phone (scheme **d**) were rendered through the freely available 3D molecule structure/viewer App (the concerned logo and the name appeared in the iphone's App store is cropped and pasted here (scheme **c**)) updated by the Apple Inc. Exactly same type models in the 2D and 3D axes can be visualized through other different Apps available freely under the name iSpartan, Molecule Simulator, Atomify, Alchemie Animator Chemistry, ModelAR: Organic Chemistry, AR VR Molecules Editor Lite, etc.

Since the ongoing rapid development of computational and theoretical chemistry is dramatically accelerated by the machine learning models, and the associated chemical & molecular graphics, the frequent computational call and implementation of them for molecular modelling such as building, sketching, representing, manipulating, developing, & analyzing trial molecular models and prototype structures [10, 11], and for predicting reaction dynamics of the molecular compounds [12−14] have incrementally raised the standard of these disciplines in the world of chemistry. Through the chemical & molecular graphics tools, the entirely new and the most potential phase of the quantum mechanical QSPR/QSAR based studies are opened up on the basis of which sometimes experimentally impracticable and unrealistic physicochemical properties of the molecular compounds such as kinetic stability, intensity to take part in the chemical reactions, ionization potential, electron affinity, electronegativity, chemical hardness & softness, electronic chemical potential, electrophilicity, nucleophilicity, charge transfer reactions, etc. can be predicted quantitatively at an exceptionally low computational cost [15−18]. Due to the promising graphical features, theoretical/computational chemists are able to mimic the behavior of the molecular systems ranging from simple to giant biomolecules and material assemblies [11], to understand the conformational properties of the biomolecules in the solution, and to trace the structural orientation of the complex protein assembly systems for the specific site interactions, functional site location, docking of the molecules, etc. [19]. Beside this, various 3D graphical features are accepted as the most impressive & magnificent computational tools in the main stream of theoretical chemistry; complex MD simulations where natural dynamic motion of the: (a) complex molecular assemblies is simulated for understanding the temporal behavior of the molecular systems [20], (b) amphidynamic molecular crystals is simulated for investigating the amphidynamic behavior [21], (c) surface mounted molecular rotors is simulated for understanding the effect of alternating electric field on their rotation [22], (d) advanced functional materials is simulated for visualizing the way in which simple molecular machines can be operated [23], and many more. After all these significant achievements of the computational/theoretical chemistries, the underlying hero, smarter, and splendid tools & techniques are none other than the advanced computer graphics aided molecular visualization and manipulation chemistry softwares out of which *ChemDoodle*, *Gromacs*, *Avogadro*, *Hypercube*, *BIOVIA Draw*, *GaussView*, *Jmol*, *MolView*, *ChemSketch*, *Molden*, and *Visual Molecular Dynamics* (VMD) are being extensively used worldwide [24]. Despite the availability of several graphical softwares hosting unique potential features, this short article presents a simple way the hierarchy of *Molden*, *GaussView*, *Jmol*, and *VMD* based molecular modelling, visualizing, and manipulating features that are in the frequent choice of the present author mainly for designing prototype molecular models & trial molecular structures, displaying equilibrium molecular structures & geometries in the 3D space, visualizing electron density based molecular orbitals including HOMO and LUMO, studying MD simulation of the complex crystalline and non-crystalline molecular assemblies, investigating the superconductivity of the doped and undoped nanomaterials, searching the sequential hydration mechanisms step by step, analyzing the MD & time series trajectories computationally, retrieving the live movies of the simulating systems & other theoretical computations, predicting the HOMO −LUMO orbitals & their Eigen values based QSPR/QSAR electronic physicochemical properties of the wide ranged molecular/ionic systems, etc. The structure of this paper is organized as follows: the Materials, Methods, and Discussions are outlined in section 2, and the specific Summary and Conclusion are presented in section 3.

II. Materials, Methods, And Discussions

Present author explicitly uses the following computer graphics aided molecular visualization and manipulation software packages mainly for the safe handling, and pre- & post- processing of the quantum chemistry program datasets. All of them were actually employed computationally in order to assess mostly the human unreadable molecular wavefunction based datasets that were either stored electronically or derived lively through the quantum mechanical computations that might be terminated abnormally or on the fly.

1. Molden

After the successful release of MOLecular electronic DENsity based graphics MOLDEN by Gijs Schaftenaar in 1993, it has been playing very critical roles in chemical and molecular graphics aided computational interpretations of the quantum chemistry calculations [25]. Despite its design and stable release of *Molden6.9* version as an efficient pre- & post-processing computational tool compatible for the Windows OS X Linux operating system, the *Gaussian*, *Gamess*-US/UK, and many other semi-empirical programs utilize it as a powerful vendor mainly to compute electronic structure based molecular properties such as electrostatic potential (ESP), ESP-charges, molecular orbitals (MOs) & their contours, and the spatially distributed variable electron density as well as to visualize their either lively run, suddenly interrupted or normally terminated outputs of the

geometry optimization & frequency calculation jobs, and to animate the concerned reaction pathways of the complex chemical reactions. In many of the computational and theoretical research steps, the Molden tools are most immediately preferred mainly for the immediate examination of the *ab-initio* convergence criteria, inspection of the ongoing calculations, tracing of the saddle points, local & global minima on the 3D potential energy surface (PES), identification of the Eigen values corresponding to the particular intermittent, recurring, & converged equilibrium geometries, extraction of the iterative Cartesian coordinates, determination of the concerned structural descriptors, analyses of the molecular geometry in the 3D space, etc. Unlike Gaussian, Inc. released graphical interface *GaussView*, the Molden bestows an additional advantage due to which different types input and output file formats of the *Gaussian* electronic structure calculation packages are accessible. Moreover, in terms of its design, features, operations, services, and software interfaces, it is a user-friendly chemical graphics that can be called easily and promptly through the commands: "*molden &"* for opening its window, "*molden test.com*" and "*molden test.log*" for loading and visualizing the input and output files respectively, etc.

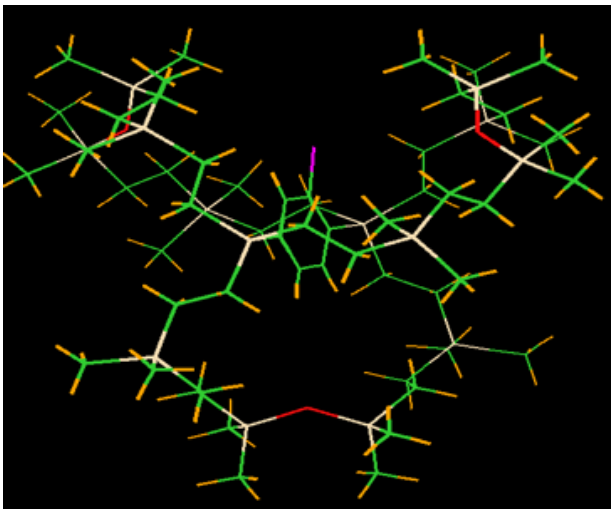


Figure 1. The Molden displayed equilibrium structure of the Si-based amphidynamic type molecular rotor with a chlorine substituent on its central phenylene ring in a wireframe model. It is an image appeared after accessing the normally terminated Gaussian *.log* file through the Molden. Exactly same visuals are appeared while reading the *.log* file obtained from the ongoing computation. This type sketch is most frequently displayed by the users, and is mostly used for checking whether the ongoing computational procedures are run normally or not, and for inspecting Gaussian in-built specific convergence criteria & their variations with the ongoing optimization steps. This wireframe model always helps the chemists/ modelers to identify where the specific parts, fragments, and elements can be placed in order to design/develop a complete prototype molecular model. It also gives the immediate views of the types of atoms, their connections, and bonds, angles, & dihedral angles associated with them. The Molden is very much sensitive to the Gaussian produced Cartesian coordinates of the atoms, and any misleading coordinates are detected & displayed in the form of scattered bonds/molecular fragments so that users can redesign and resubmit the specific computational jobs efficiently and promptly.

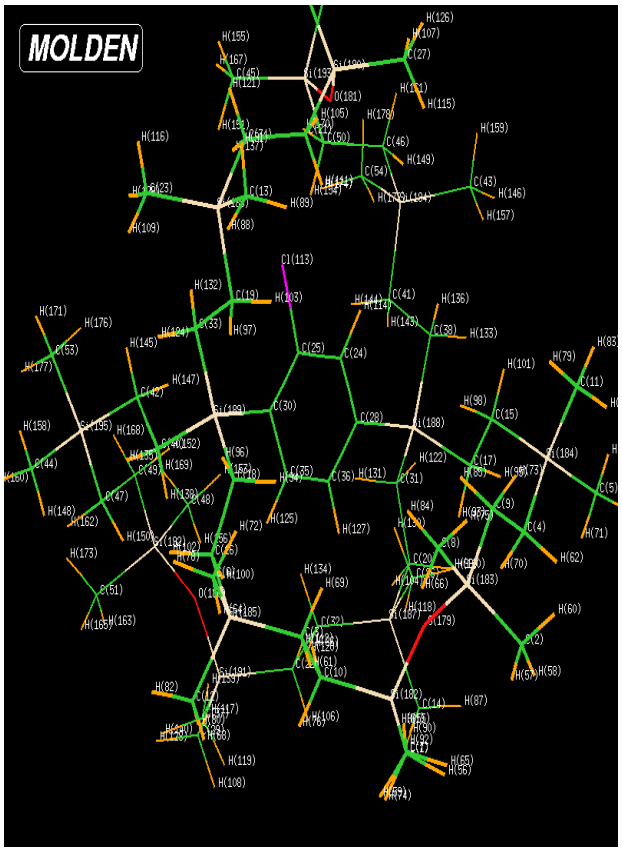


Figure 2. The Molden displayed molecular structure near the transition state (TS) of the Si-based amphidynamic type molecular rotor with a chlorine substituent on its central phenylene ring in a wireframe model. It is an immediate image appeared after accessing the Gaussian derived transition state *.log* file through the Molden. All the atoms were labeled through the "*Label*" feature of the Molden. This wireframe sketch is most frequently displayed by the users, and is actually used for checking whether the ongoing computational procedures are terminated normally or not, and for identifying the atomic connections explicitly. It is used to visualize the immediate views of the local, global, and the saddle point structures designated with and without negative Eigenvalues. The Molden is highly sensitive to the Gaussian produced Cartesian coordinates of the atoms, and any misleading coordinates are detected and displayed in the form of scattered bonds/molecular fragments.

The pop-up window that appears after clicking the *Geom.conv* button on the Molden panel explicitly produces all the convergence criteria both in the form of human readable datasets and graphical sketches for the normally run, suddenly stopped, and abnormally terminated calculations. In addition to this, the Molden is equipped with the facility of: visualizing single and multiple unit cells of the crystal from the Cambridge Structural Database, Z-matrix editor for building and specifying trial molecular geometries, pre- and post- processors, etc. Present author uses almost all these features of the Molden out of which few are demonstrated in the Figure 1 to Figure 4 where the specifically mentioned captions describe what the figures are all about and their major significance & applications in quantum mechanics based theoretical computations.

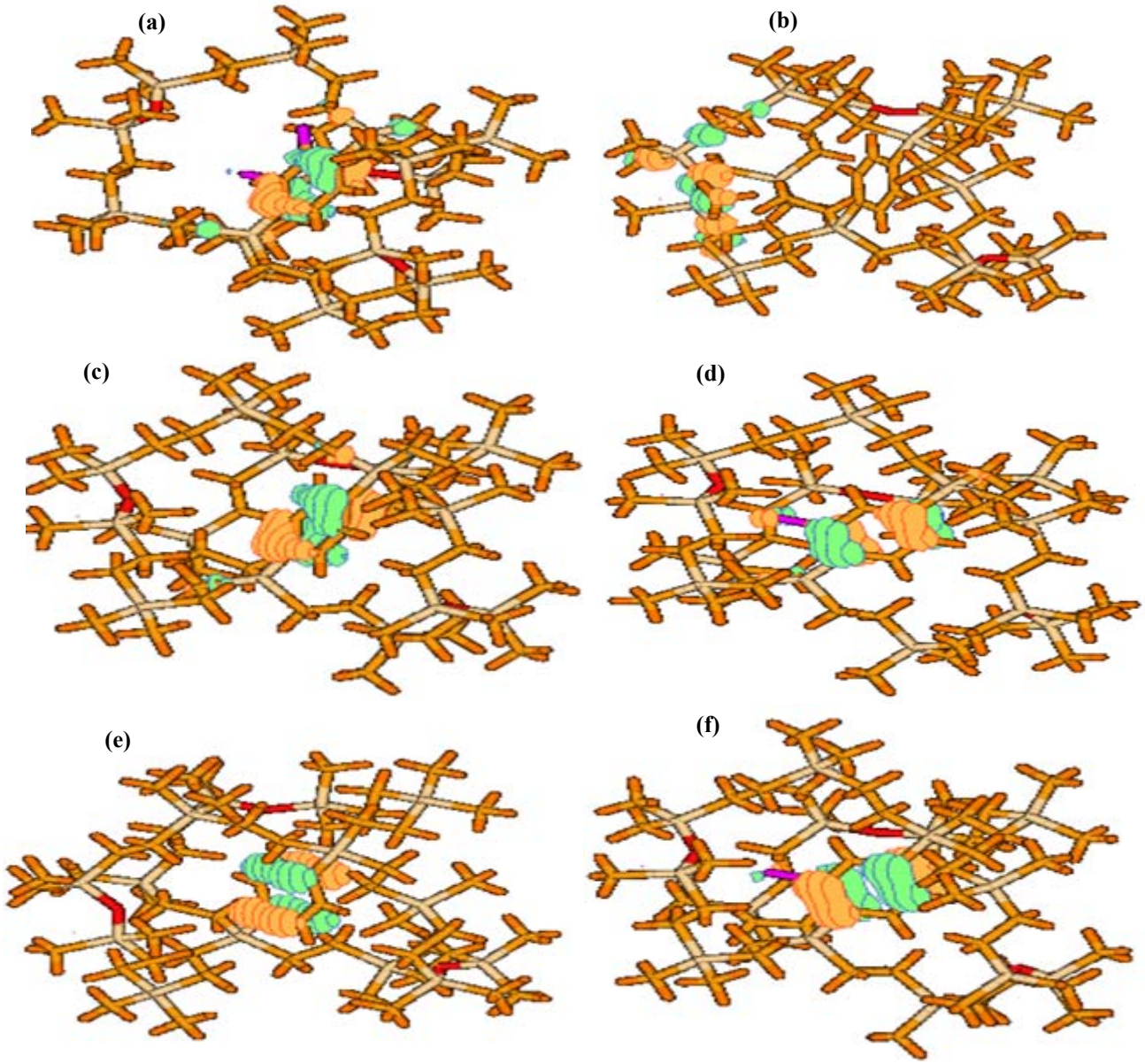


Figure 3. The Molden displayed molecular orbitals (MOs): (a) molecular orbital (occupancy = 2) with two Cl atoms, (b) highest energy alpha orbital (occupancy = 1) of the cationic form without halogen atoms, (c) HOMO (occupancy = 2) without halogen atoms, (d) HOMO (occupancy = 2) with a Cl atom, (e) vacant beta orbital (occupancy = 1) of the cationic form without halogen atoms, (f) vacant beta orbital (occupancy = 1) of the cationic form with a Cl atom, on the central rotating unit of Silicon based amphidynamic crystal. For simplicity, all the atoms and the covalent bonds are displayed in a "Tube" model feature of the Molden. The concerned immediate views of the MOs were extracted from the Gaussian derived molecular wavefunction based human unreadable datasets through the special MOs visualizing features of the Molden. Unlike in the wireframe models (Figure 1 and Figure 2), the tube model feature uses a small tube to display the bonds and the atomic positions so that the molecules can be manipulated & visualized conveniently on the computer screen. This type model shows molecular alignments in the 3D axis with the exact location of the atoms, bulky groups, atomic bonds, distances between the atoms & bonds, angles between the three bonded atoms, dihedral angles between the four bonded atoms, axial and equatorial bonds, precise orientation of the vector or bond of the molecule parallel to the Cartesian axis, etc.

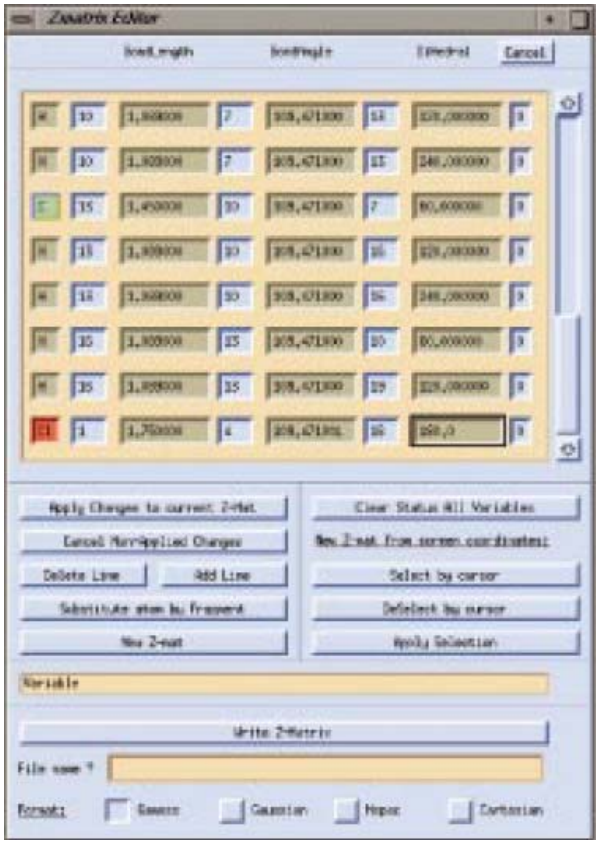


Figure 4. The Z-matrix editor pop-up window (screenshot) of the Molden displaying corresponding Z-matrix and the edit-controlled buttons. The concerned Z-matrix of the molecular compounds in the *Gaussian/Gamess -US/UK* package readable format can be extracted and used directly as their input files. It is an essential feature of the Molden easing trial-molecular structure build-up processes, connectivity descriptions of the atoms, & molecule editing tools, and supporting the Cartesian coordinates generating sources. It is mainly used to substitute atom by fragment, to adjust the bond angles, dihedral angles, & bond lengths, and to achieve a desired molecular symmetry step by step. The concerned Z-matrix with the atomic connectivity for the small prototype molecules can be constructed stepwise manually (just by using hand and mouse), but for the larger molecules, this manual construction becomes impractical, boring, and tiresome. The dedicated Z-matrix features can be used comfortably for the latter.

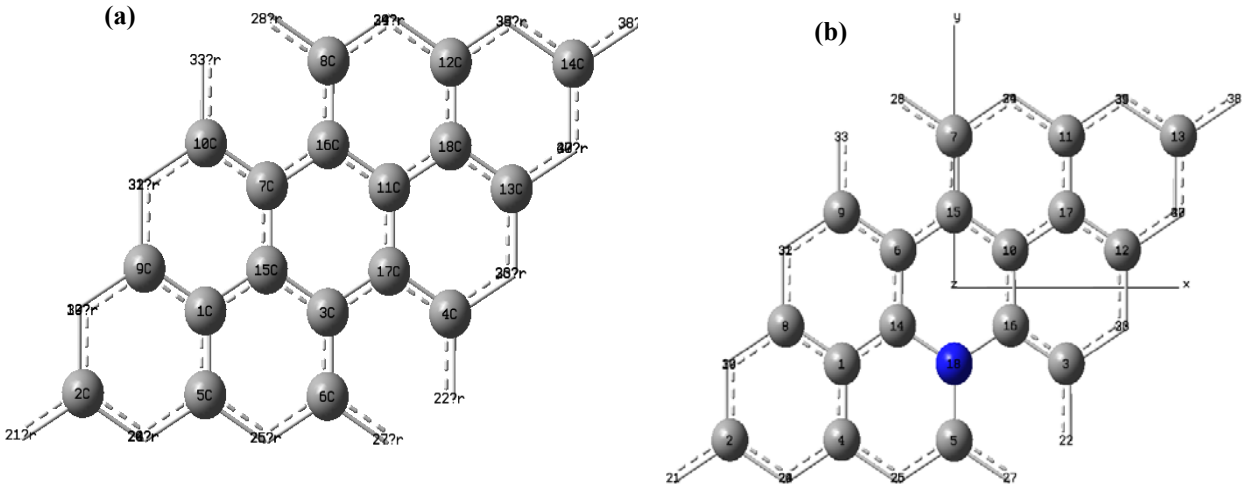


Figure 5. The GaussView displayed DFT derived unit-cell geometry of the (a) undoped and (b) Nitrogen-doped monolayer graphene sheet. The grey and blue colored spheroids represent C and N atoms, respectively. All the atoms are labeled using "*Labels*" feature of the *GaussView*. The 3C atomic spheroid of the prototype model (a) was doped by a Nitrogen atom, and the respective Cartesian coordinates with *.xyz* extension were extracted explicitly prior to apply DFT method. The resonating behavior of the electrons (electronic delocalization) inside the graphene network is also clearly rendered with the GaussView feature. The same model can be used to assign the Mulliken derived partial atomic charges and their specific distributions explicitly to each and every atom. The two dimensional honeycomb structure of the carbon atoms with SP^2 hybridization can also be confirmed from the in-depth structural analysis of the same display. The detailed comparison in the geometry of the honeycomb rings and the entire electronic properties including exceptionally high conductive properties before and after doping N atom can also be easily interpreted and examined. The same models can be used to inspect the geometrical distortions of the honeycomb rings after doping N atom into the prototype model of the graphene layer. As per the Ref. [31], the Vienna *ab initio* simulation package (VASP) uses the same type model as its prototype structure to simulate the monolayer graphene sheet under periodic boundary condition (PBC). The atom and the plane centered rotation feature of the *GaussView* can be used to visualize this layer on *XY*, *YZ*, & *ZX* planes. This image is reproduced from the research paper of the same author Ref. [29].

2. GaussView

With the initial release of *Gaussian* orbitals based electronic structure computing software package in 1970s by John Pople, the continuous updating, developing, and releasing of it with the complete incorporation of progressive quantum chemistry tools & techniques has been licensed and prosecuted by the Gaussian, Inc. since taking its ownership in 1987 [26]. In order to execute all the Schrodinger wave mechanical equation related computational outputs, human unreadable complex datasets, and the entire molecular wave function based computational procedures, the Gaussian, Inc. has been iteratively releasing various spectacular versions of the possibly most advanced and powerful computer graphical interface namely *GaussView*. One of the main reasons of its high preference and likeliness among the theoretical, computational & experimental laboratory instructors, teaching and research faculties, chemists, scientists, students, research fellows, etc. is due to offering exceptional chemical & molecular graphic features compatible with the Gaussian run quantum mechanical calculations & wave function based numerical derivations, and bestowing the most superb molecular-modeling techniques side by side with the facility extending to the direct insertion of the biological fragments such as alanine, arginine, cysteine, etc., cycloalkanes type closed-chain organic compounds, and the C_{60} type fullerene cluster. It is advanced computer graphics aided molecular visualization and manipulation software that helps them not only in creating Gaussian input file formats, in enabling the direct run of the Gaussian calculations without any command line instructions, in monitoring the ongoing computations in accessing the Gaussian produced output file formats, in acquiring, retrieving & visualizing the molecular wavefunction based chemical bond information from the Gaussian derived human unreadable datasets, in interpreting the various electronic properties and electron density based AOs' & MOs' features, in animating the different vibrational modes but also in depicting and comparing the combinational or individual type vibrational, IR, Raman, and NMR spectral patterns, etc. The latest released of *GaussView* version 6.1.1 has more additional features with the

special treatments on fixing almost all the computer bugs that were encountered in the versions 6.0 and older mostly while handling the Gaussian package produced quantum chemistry results such as anharmonicity and anharmonic frequency analysis, solvation cavity, optical rotations, and optical rotary dispersions, vibronic spectral interpretations, retrieving & saving the live movies of the various Gaussian computations, and setting up of the special type Gaussian jobs such as multi-job setups, call, & run, conformer search, symmetry & brushing tools, etc. [27].

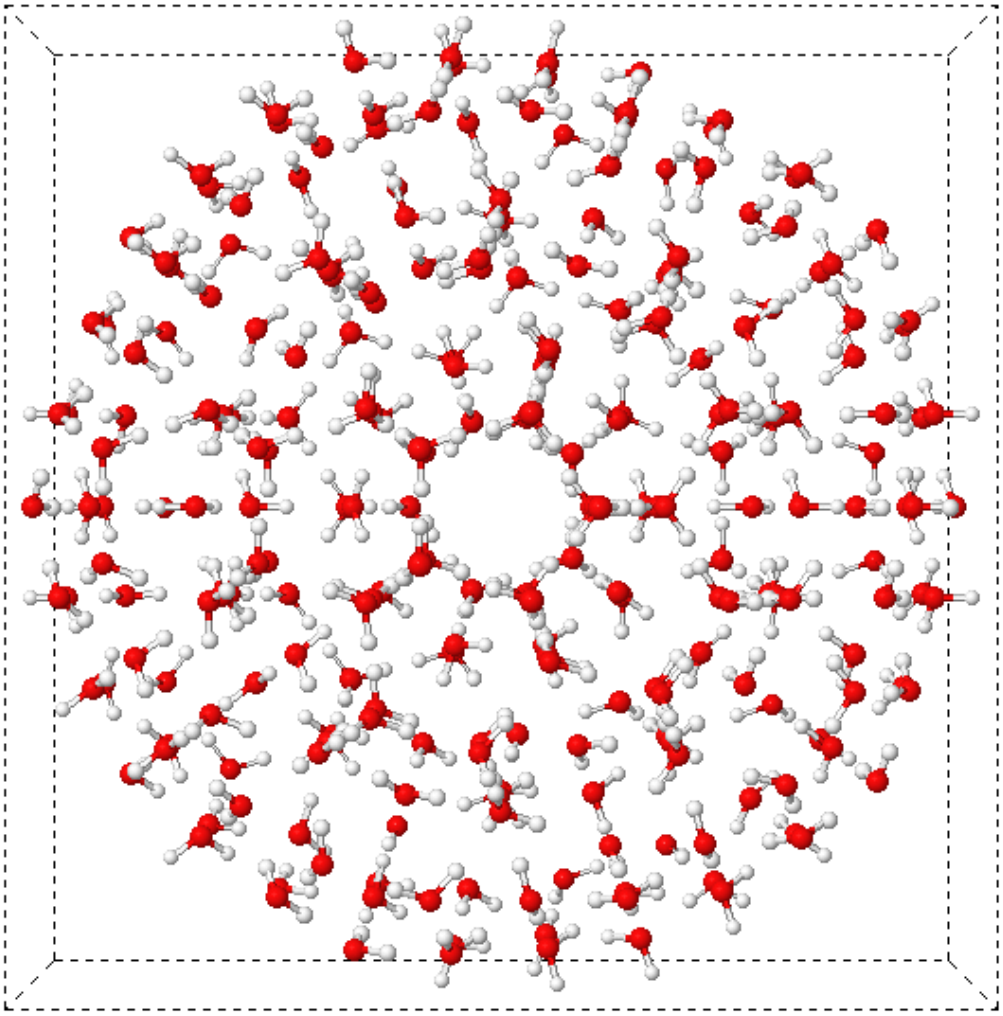


Figure 6. The *GaussView* displayed water molecules confined into the definite boundary box; a discrete hydrogen bonded assembly of the 280 molecules equivalent of H_2O. The white, and red spheroids represent H, and O atoms, respectively. This magnificent view describes how actually the 280 molecules equivalent of H_2O are aligned in three dimensions, and interacted to each other while attaining the stable hydrogen bonded structural network. It is equally applicable to interpret their preferences & possibilities of taking part in H-bonds formation, to visualize the exact abstract image of the water in the liquid state, to extract the ordering tendencies/patterns of the H_2O molecules, to understand the water network modeling & analysis, to study the micro structure, dynamical, & electronic properties of the bulk water at wide range temperatures, to analyze the radial & angular distribution functions for water through molecular visualizations, to study the anomalous properties of liquid water, to compare the theoretically predicted & experimentally measured physicochemical properties for liquid water, to permit direct quantitative study of the isotope effects exhibited by the liquid water & aqueous solutions, to evaluate the long range molecular interactions into the bulk level, to explain the H-bonding structures & their influences on dynamical properties of the liquid water, to disclose the effect of an electric field on dynamical and structural properties of liquid water, etc. It is an image extracted from one of the ongoing research projects of the present author.

With all these potential practical applications, present author is very much handy, and familiar with the features presented in the *GaussView* version 5.0.9. Despite integrating many more improvements and the spectacular features into its newer versions, the *GaussView* 5.0.9 is still equally workable and functional on Windows, and applicable to almost every phases of the computational and theoretical researches that are aimed to study the wide ranged molecular systems such as building, visualizing, & manipulating targeted molecular structures, importing & displaying the molecules from the PDB file formats, editing & modifying the advanced structural features, setting up the ONIOM type computations in Gaussian, extracting & viewing the summary of the results in the form of graphical plots, sophisticated modeling & animating features of the excited states, displaying splendid views of the AOs, MOs, frontier MOs, & their electron amplitudes (contours) with electron density interactions, extracting the MOs' Eigen values explicitly from the Gaussian produced human unreadable datasets, generating highly resolved scenes of the dynamic chemical reactions & their mechanisms, etc. [27, 28]. Since this molecular & chemical graphics offer tremendous applications and commendable features, it is not possible to cover all of them here. But, present author still thinks to underscore herewith the importance of some of the GaussView 5 generated snapshots of the simple to complex molecular systems that lie under his current research interests which not only attracts the interests of the beginners but also promotes its frequent uses in the multidisciplinary academic fields. The GaussView rendered spectacular visuals are displayed in Figure 5 to Figure 10 where the precisely mentioned captions describe what the figures are all about and their importance in computational chemistry, quantum chemistry/physics, theoretical chemistry/physics, chemical kinetics & complex reactions mechanisms, and drug discovery science.

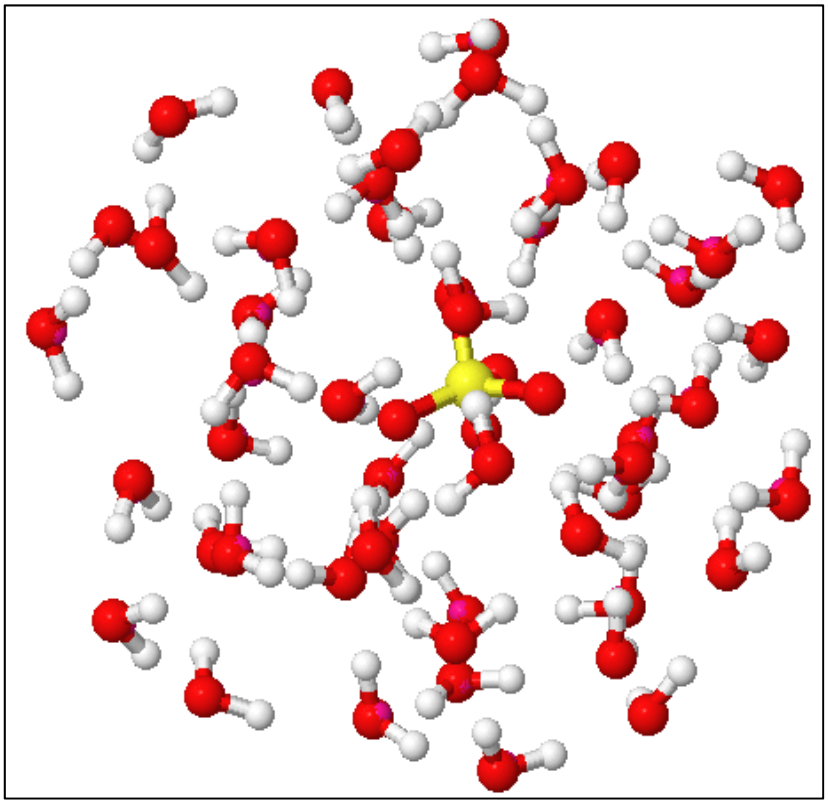


Figure 7. The *GaussView* displayed ionic hydration model of the $[SO_4^{2-}(H_2O)_{50}]$ cluster with hydration number n = 50. The white, red, and yellow spheroids represent H, O, and S atoms, respectively. This close view describes how actually the constituent particles are aligned in the three dimensional space, and interacted to each other while attaining the stable structural entity of the hydrated ionic network. This type model is useful to understand the characteristic properties of the ionic compounds in the aqueous type solutions, to inspect which of the H_2O molecules are connected to the dissolved ions through H-bonding, to realize the ion-dipole forces that can establish the stable ion-water cluster, to speculate the hydration shell around the ions, to determine the dynamic hydration number for the biologically important ions, to reveal the information regarding the structure of water beyond the first hydration shell, to approximate the hydrogen bonding numbers of the solvated H_2O, to predict the experimentally immeasurable properties through molecular dynamics simulations, to get the quantitative differentiation between the coordination number and hydration number of the solvated ion, to achieve the qualitative insights and microstructure of the aqueous type electrolyte solutions with dissolved ions, to estimate the solvation enthalpy ($\Delta H_{hyd.}$) of the ions, to consider the orientation distribution (hydration factor) of the H_2O molecules around the specific ions, to visualize the hydration shell & H_2O-dipole ordering/disordering patterns, to investigate the ionic transport systematically & sequentially, to reveal the image of fine structures at the solute-solution interface, etc. It is an image extracted from one of the ongoing research projects of the present author.

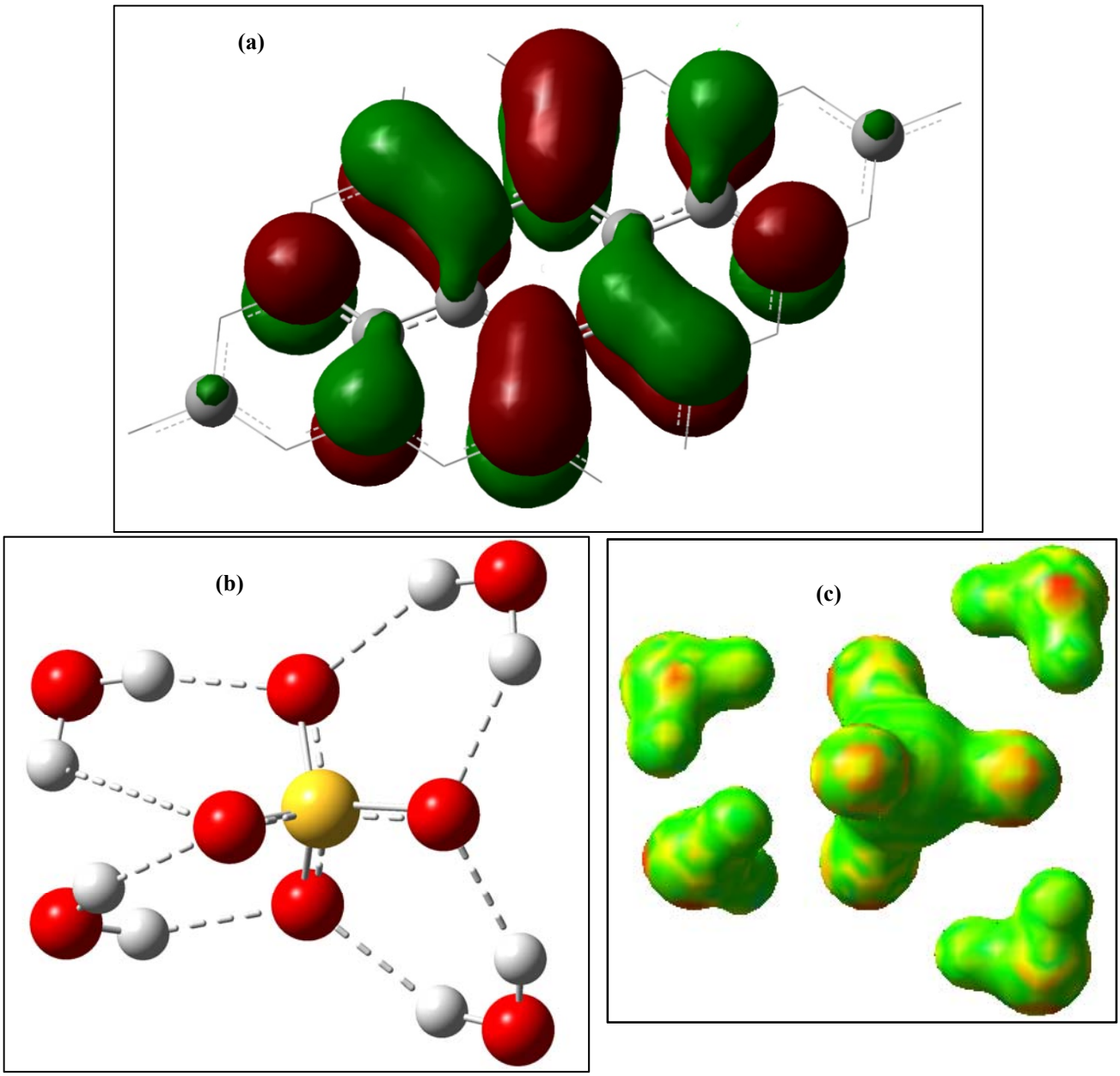


Figure 8. The *GaussView* displayed DFT derived (a) HOMO orbital of the undoped monolayer graphene sheet explaining orbital parity, delocalized electron density, animated views of the electron density & wavefunction, atomic nuclei concentrated molecular orbitals, etc. The HOMO-LUMO orbitals representations and their DFT derived *Eigen* values are actually useful for QSPR/QSAR studies, kinetic/chemical stabilities, superdelocalizability, etc.; (b) H-bonded equilibrium molecular geometry; and (c) Electron density surface (ESP) mapping, of the tetrahydrated divalent sulfate $[SO_4^{2-}(H_2O)_4]$ ion. The white, red, and yellow spheroids represent H, O, and S atoms, respectively. These splendid visuals respectively describe the spatial alignment of the electron density lobes of the graphene HOMO orbital, symmetrical configuration of the centrally located SO_4^{2-}-inbound four molecules equivalent of H_2O, and depict the actual orientation & location of the four H_2O molecules in the immediate surrounding of the SO_4^{2-} ion where the orientations (interwater gap) of the electron density surface of the nearby H_2O molecules are clearly shown, assuring no possibility of developing interwater H-bonds as indicated by the experimental tools and techniques. Mostly, this diagrammatic sketch allows the thorough examination of the experimentally observed hydrated ionic moieties in the light of H-bonding. All these images are extracted from the research papers of the present author Ref [29] & [30].

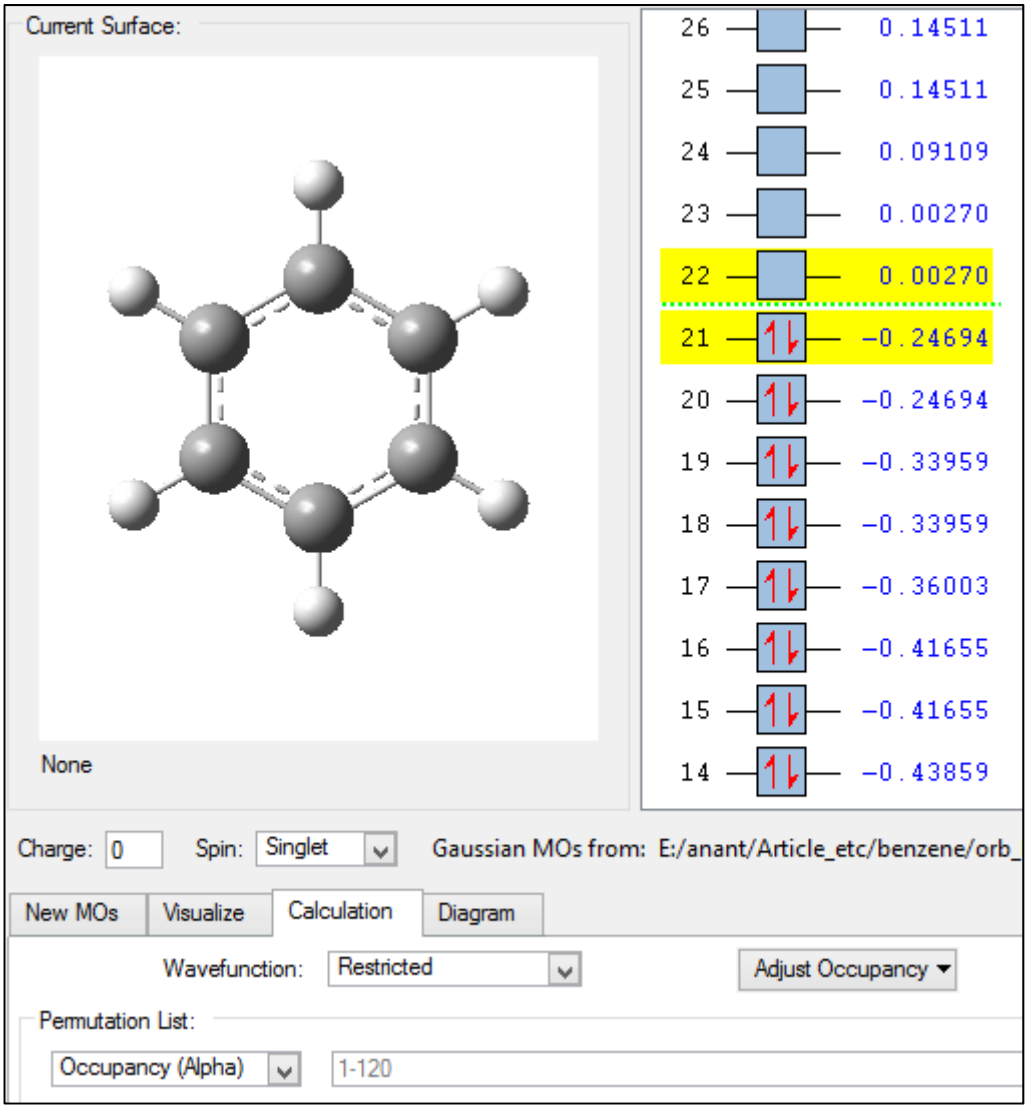


Figure 9. The MOs editor pop-up window of the *GaussView* displaying corresponding MOs with and without electron occupancy and the edit-controlled buttons. The HOMO and LUMO orbitals are always displayed with yellow colored highlights by default, and all the MOs lying below to the HOMO and above to the LUMO are arranged in increasing order of their quantum chemistry derived Eigen values in *a. u.* scale. Unlike in Molden, this feature of the GaussView offers extraordinary advantages more especially while retrieving the electron density of the MOs and chemical bonds, total electron density surfaces of the molecules, electrons' amplitudes measuring three dimensional contour plots and lines, MOs isosurfaces & their explicit contours, alpha electron density surfaces, and the ESP mapping of all the occupied & virtual MOs. It is an important feature of the *GaussView* summarizing all the calculation options for the restricted and unrestricted wavefunctions, visualization options of all types MOs, and a new *.chk* file generating or the existing *.chk* or *.fchk* file loading options of the Gaussian, permitting the prompt resubmission of the suddenly abnormally-terminated computational jobs at the limited computational resources such as memory space, data saving storage, Gaussian used dynamic memory, and limited number of cores, etc. It is a screenshot image of the GaussView 5.0.9 MOs surface viewer features.

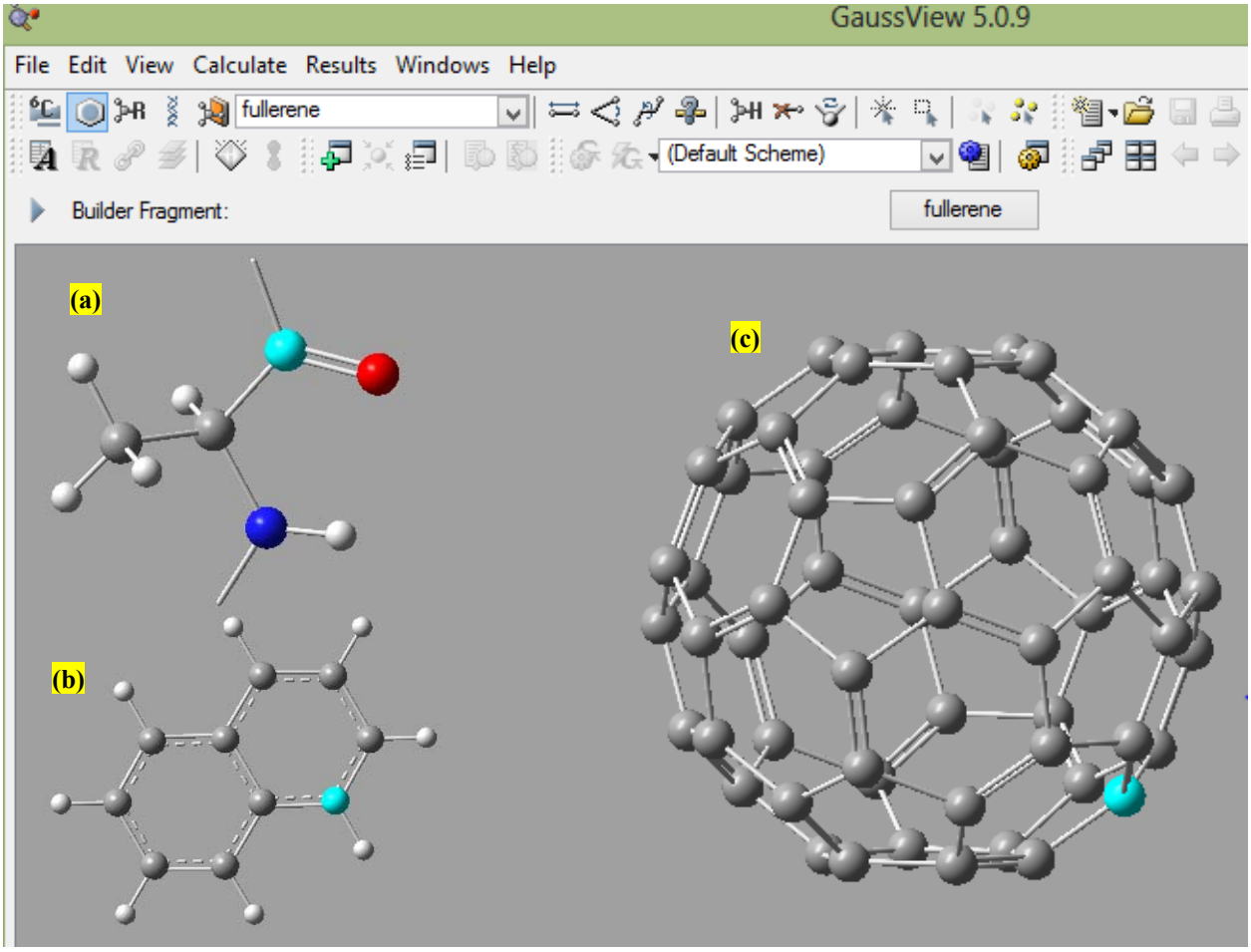


Figure 10. An example of the large molecular fragments (a) biomolecule (alanine, as an example), (b) naphthalene type aromatic rings, (c) fullerene type carbon clusters, etc. inserting facility of the *GaussView*. This special feature facilitates the building up process and atom-fragment join methods of constructing trial molecular geometry and a prototype structural module of the giant biomolecular systems & the host-guest clathrate type macro-caged molecular compounds, allows the direct placement of the fragments into the most active sites of the receptor, eases finding out the route way for the complex chemical reactions, coordination complexes, chemical synthesis, & drug discovery, acts as a base for understanding the fundamental principle of the "click-chemistry" & as a principal tool for predicting the reaction routes of the organic synthesis, helps modeling the interactive peptide chains, provides a direct tool for phasing the X-ray diffraction data, creates a polymer chain step-by-step through the visual inspections, develops a giant molecular system by chopping up the initial molecular model sequentially, acts as a key tool in Gaussian based fragment guess calculations, counterpoise calculations, etc., serves as a source for representing molecular graph applicable to the artificial intelligence (AI), drug discovery & cheminformatics, behaves mostly as a direct computational mean for the routinely analysis of the molecular structures, their comparisons & structural validations, etc. This is an integrated image of the few screenshots of GaussView 5.0.9 builder fragment features.

3. Jmol

As per the information released to the public at Jmol homepage [32], the computer programming targeted to create the Jmol software was actually began with the advanced and new innovative thoughts by replacing Minnesota supercomputer center owned XMol molecular visualization package, the then unmaintained and outdated software version existing without making availability of its source codes to the probable users. The principal originator Dan Gezelter was involved initially in order to amend the few major problems, issues, and software bugs faced by the XMol without excluding its major visualization & manipulation features, but with incorporating even more advanced functionalities, and he could eventually develop its first version replacement tool in 2001 as Jmol. Since then, it is serially released in different modified and stable as a free open been versions that are made available to the chemists, educators, researchers, and molecular modelers as an open source Java based

graphical viewer [33, 34]. It is uniquely developed on the Java language programming codes with sufficient advanced features for the chemicals, crystals, materials, and biomolecules without any hardware requirements [32-34]. It is a very user friendly high performance three dimensional rendering tool that can support all the main computer browsers such as Microsoft edge, Internet explorer, Firefox, Safari, Google Chrome, and Opera, and can be run easily on the Java installed operating systems macOS, Windows, UNIX, and Linux, with the auto-adaptation of their in-built languages. Exactly saying, the Jmol package offering compressed "binary.zip" file with "Jmol.jar" is an easily executable application module on the Java-installed portable disks even without its full installation. By running the *jmol.jar* module computationally, users may get direct access to the various type human readable/unreadable chemical file formats with the *.pdb*, *.cif*, *.mol*, *.cml*, *.xyz*, *.csf* extensions, and GAMESS, Gaussian, Amber, ADF, & MOLPRO produced outputs, etc. More particularly, the Jmol bestows many more potential advantages over other computer graphics aided rendering tools: (a) it executes the files of the Cartesian coordinates of the atoms with 'EP' as the atom with a zero nuclear charge meaning a dummy, nonexistent atom (Figure 11(a)) and without any dummy atoms (Figure 11(b)); (b) it reads the files with the MODELLER generated model with HETATM residues (Figure 11(c)) & connected chain of the atoms (Figure 11(d)); (c) it offers an alternative to the chime plug-in used by the web browsers while displaying 3D structures of the molecules [35], (d) it executes the files that are dragged and dropped into the "*Jmol.jar"* application window directly, (e) it opens the file formats with MOPAC and Molden created Z-matrix datasets (Figure 11(e)), (f) it supports for the unit-cell and symmetry operations of the crystallography, (g) it even creates the Gaussian input file formats, but unable to read the Gaussian output file (but it does recognize the file type correctly), to reformat the Gaussian generated *.chk* files to *.fchk* files, and to read the later explicitly, (h) it offers many additional features such as measurements, distance, vibrations, animations, bounding box, electron density surfaces tools with solvent and solvent-accessible surface kits, spectral displaying tools, etc. (Figure 11(g), Figure 11(h), Figure 11(i)). Besides these, the Jmol offers tremendous graphical applications and commendable features on prototype molecular building up processes, molecular visualizations and manipulations, crystallography featuring unique rendering skills of the unit cell geometry inside the boundary box with and without lattice parameters & unit cell boundary conditions, etc. Herewith, present author mainly stresses the importance of these features-incorporated scenes of the Jmol rendered images (Figure 12 and Figure 13) of the giant molecular crystalline assembly that lie under his current research interests. The crystal-clear views of them not only attract the interests of the potential users but also promote its brand for the frequent uses in the multidisciplinary fields/tasks of the science, technology, and engineering. Each specific caption of the figures describes the real and in-depth necessities of these magnificent views of the molecular and crystalline assembly to interpret the quantum chemistry results quantitatively.

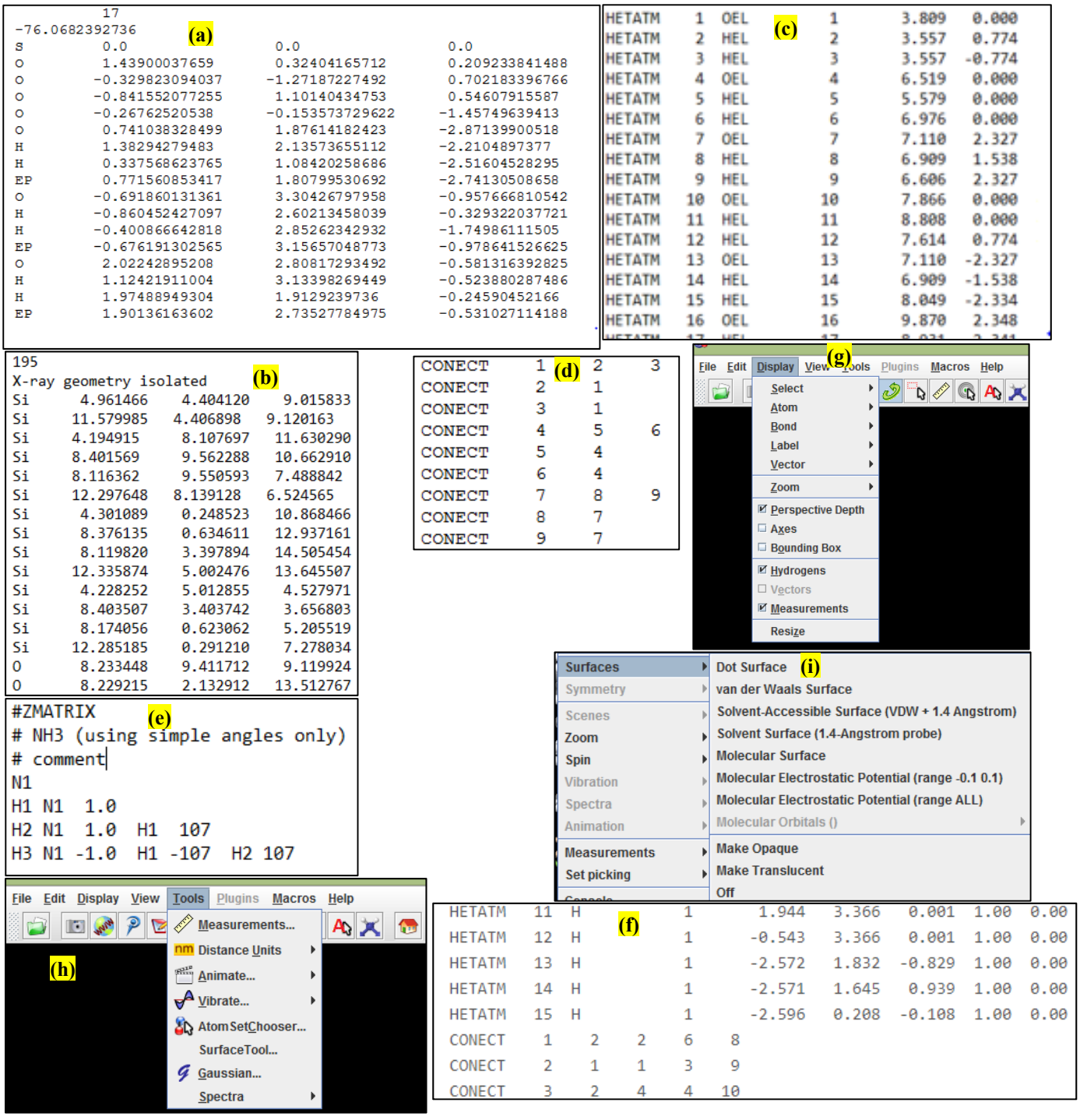


Figure 11. The Jmol readable file formats with (a) Cartesian coordinates of the atoms with 'EP' as the atom with a zero nuclear charge meaning a dummy, nonexistent atom; (b) Cartesian coordinates of the atoms arranged in the rows and columns; (c) MODELLER generated model with 'HETATM' residues on the top with (d) connected chain of atoms on the bottom; (e) MOPAC and Molden created Z-matrix datasets; (f) *pdb* file with 'HETATM' residues & connected chain of atoms. Unlike Jmol, there is mostly not a single program that can read all these data formats and display the corresponding molecular models in the 3D axis. The exceptional modelling features of the Jmol with (g) bounding box, crystallographic axes, unit cell dimensions, etc. are unique to study the crystal morphology; (h) measurements, animations, and vibrations tools, surface tool, Gaussian input file generator, and the spectral visualization tools ease the interpretation and analyses of the quantum chemistry package revealed theoretical results; (i) electron density surface tools with solvent and solvent-accessible regions. All these datasets were cropped from the present author's original archived researches.

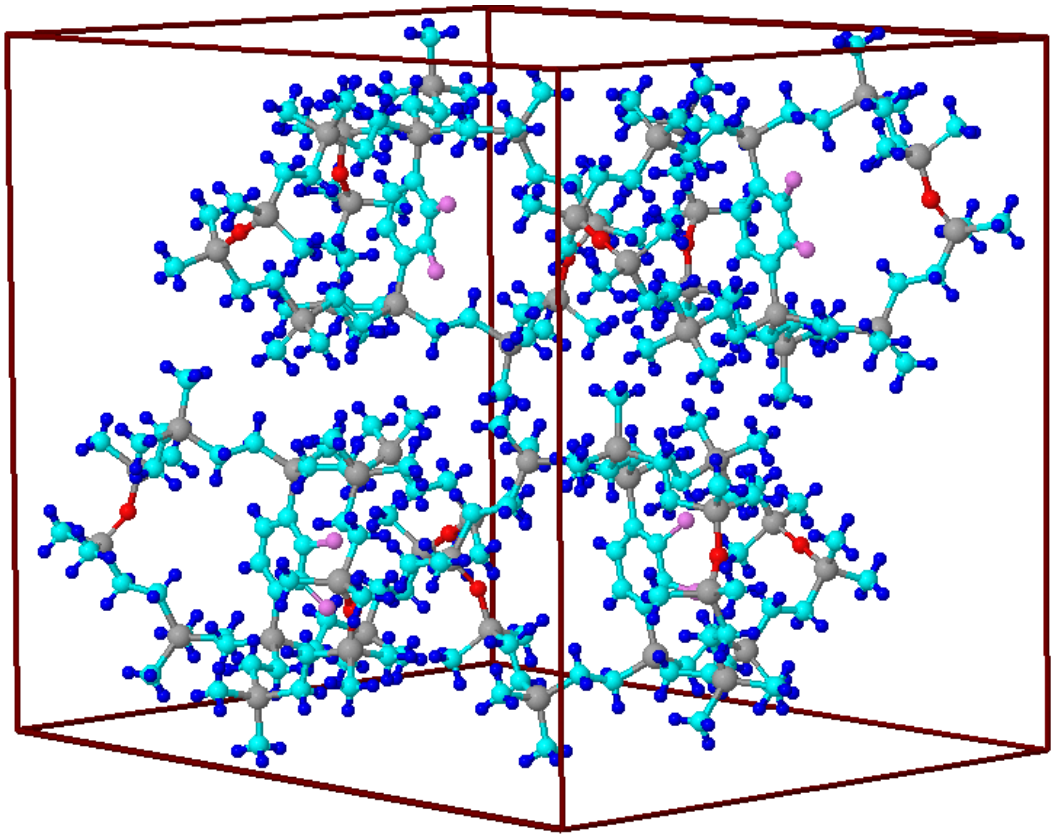


Figure 12. A Jmol generated unit-cell structure of the amphidynamic type orthorhombic molecular crystal with 4 molecules per unit cell. It is an image rendered from the theoretical model (SCC–DFTB) derived unit-cell Cartesian co-ordinates of the crystalline siloxaalkane molecular gyroscope with difluorophenylene rotators. The cyan, blue, dark gray, red, and indigo spheroids represent Carbon, Hydrogen, Silicon, Oxygen, and Fluorine atoms respectively. The SCC–DFTB derived Cartesian datasets reformatted in the format of Figure 11(b) were directly imported into the "*jmol.jar*" application window, and analyzed the crystallography & crystal morphology with its rendering tools displayed in Figure 11(g) and Figure 11(h). This sort of unit-cell molecular modeling is very much useful to check the structural consistency with the X-ray derived crystallography, to measure the geometrical and topological descriptors such as bond length, bond angle, dihedral angle, molecular surface area, etc., to reveal the 3D representation of the ground state equilibrium structure, transition state, and other local-minima of the potential energy surface, to confirm the spatial alignment of the molecules & their fragments, to visualize the static and dynamic parts of the molecular machines such as motors, rotors, propeller, sensor, shuttle, tweezers, scissors, gyroscopes, & compasses, to recognize the structural topology of each and every molecules of the giant molecular systems with periodic molecular arrays, to locate the arrangement of the molecules/atoms in two/three dimensions, to idealize the unit-cell packing, lattice structure, and crystal morphology, to uniquely describe the structural motif and unit-cell symmetry, to visualize the molecular positions and their probable inter- and intra- molecular interactions, to emphasize the positional linkage between the molecules in the unit cell, to make an abstract image of the periodic patterns of the unit cells and the entire solid state crystals, to act as a prominent mean of the molecular and crystal simulations even without associating experimental datasets, etc. This image is extracted from the research paper of the present author Ref [36].

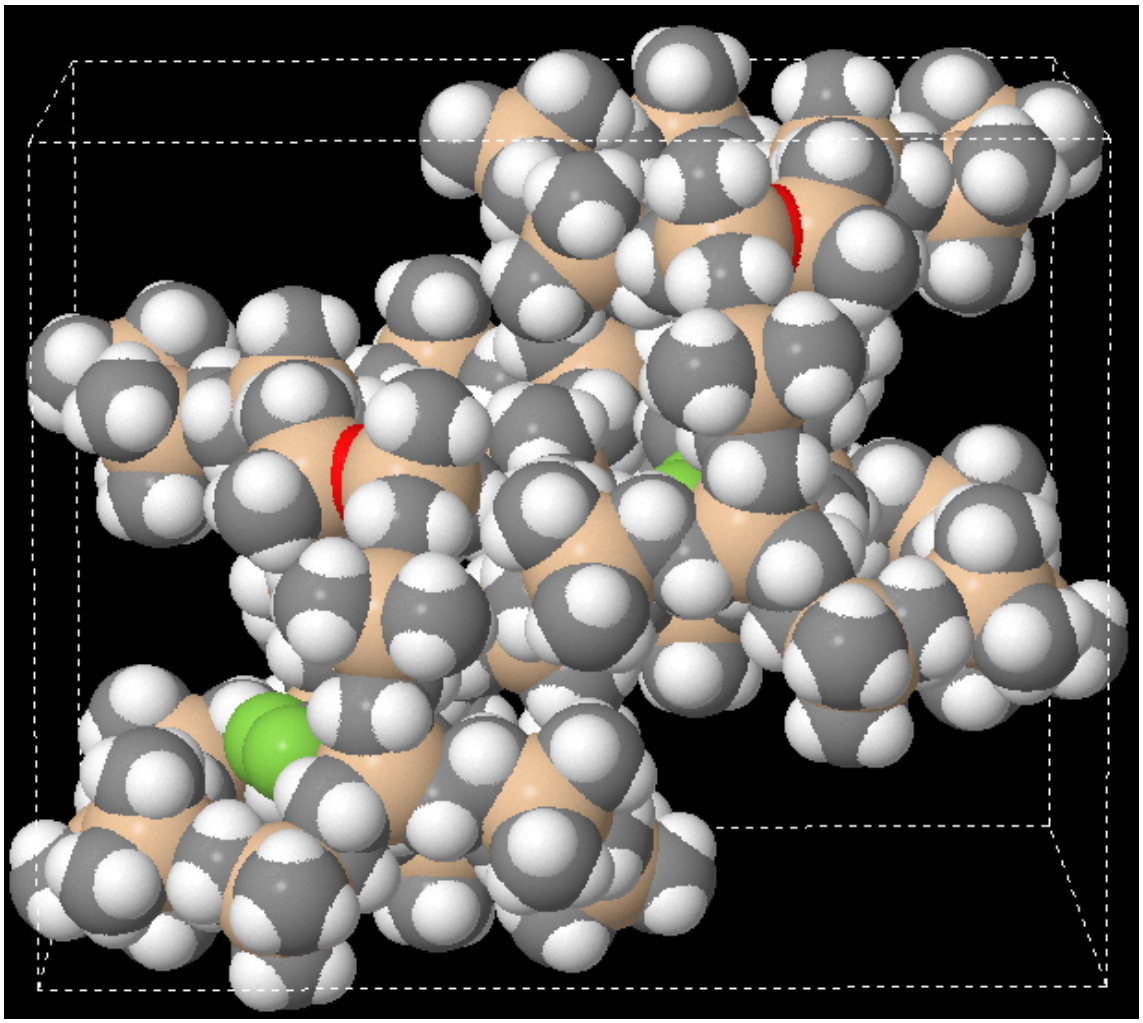


Figure 13. A Jmol generated space-filling, Van der Waal's-based representation of the unit cell structure of amphidynamic type orthorhombic molecular crystal with difluorophenylene rotator displayed in Figure 12. The Carbon (C), Silicon (Si), Hydrogen (H), and Oxygen (O) atoms are displayed in black, light-orange, white, and red colored spheroids. In quantum chemistry, a space-filling, Van der Waal's model is the most realistic 3D molecular surface viewer where the atoms are represented by the unique colored spheroids, and their radii are taken as either equal to the Van der Waals radii or proportional to the covalent radii of the atoms. This sort of magnified image is highly applicable more especially to present the abstract representation of the molecules, to confirm the molecular shapes, amount of the space molecules can occupy, and their three dimensional boundaries, to understand the molecular Van der Waal's volume and surface area, to approximate the solvation area and solvent-solute dielectric boundary, to determine the solvent accessible surface area of the biomolecules and the effective charge distributions on their surfaces relevant to binding, to map the extent to which the protein-residue is surface-exposed, to visualize the real time interactive systems, to predict the QSAR based physicochemical properties, to study the molecular interactions, to relate the bulk properties of the substances, to investigate the crystal packing and morphology, etc. The space filling model is very often used to inspect how H-bonding causes splitting of the van der Waals surfaces. Though this type graphical view is the most realistic, it makes sometime the chemists confused as the space-filler feature screens the inter-atom linkage and underlying molecular organization.

4. Visual Molecular Dynamics (VMD)

In the years between 1960 and 1990, a huge challenge was faced by the chemists, scientists, biochemists, educators, planners, modelers, technology lovers, software developers, and R & D sectors while simulating, animating, visualizing, and modeling the large biomolecular systems, and interpreting the molecular dynamics simulations derived results and their MD & time -series trajectories on the limited computational resource platforms and computing technologies, hardware requirements, data storage, CPU timing, computer memory, and the disk storage [37]. After the successful development of C++ programming code based computationally cheap, cost-effective, and high performance visualizing three-dimensional rendering molecular and chemical graphics tool, namely Visual Molecular Dynamics (hereafter, VMD) in 1995 by Klaus Schulten, William Humphrey, Andrew Dalke, and John Stone, and its fortunate compatibility to run under the macOS, Unix, Windows operating systems, the then cloud computing platforms adapted VMD has been extensively using worldwide mainly for the advanced molecular simulations, manipulations, visualizations, and molecular modeling tasks as well as for enabling the computational and theoretical chemists to achieve the most cost-compromise and the practically relevant quantum mechanical solutions of the giant, moderate, and small sized MD simulation systems with and without periodic boundary conditions, and their time-series trajectories [38, 39]. Besides being an advanced computer graphics aided efficient visualizing, modeling, designing, and manipulating software, the VMD is quite popular 3D chemical and molecular graphics tool hosting the unique features suitable for assessing the MD simulation and other potential simulation techniques produced time series trajectories containing several recurring molecular structures, and for displaying the concerned molecular model and the quantum chemistry computed atomic and molecular motion magnificently. So, unlike Molden, GaussView, and Jmol tools, the VMD has a substantial ability to render the high resolution scene of the total molecular electron density surface, molecular orbitals' iso-surfaces with ESP mappings at the comparable computational costs, and can be uniquely connected to the ongoing MD simulation tasks & other theoretical calculations so that each and every intermittent molecular coordinates can be easily loaded into its application window even without facing any extra burden of its execution in reading the manually uploaded datasets stored at the computer disk [39]. Moreover, the VMD tool has many more relatively better and advanced potential features such as (a) displaying and manipulating multiple molecular compounds at the same time, (b) visualizing and rendering the multiple views of the complex molecular systems, (c) choosing the visualization of the subset of the atoms (the atoms to be excluded in the molecular views can be controlled), (d) users' friendly rendering and coloring styles to render the scene with multicolored atoms, bonds, and molecular fragments, (e) multi-formats data file (protein data bank files with *.pdb* extension, protein structure files with *.psf* extension (created from the *.pdb* file), *dcd* trajectory files containing no information about the atoms and their connectivity, the simulator generated files with *.dat*, *.imp*, and *.txt* extensions, etc.) (Figure 14) accessing abilities, (f) mouse interacting tools with the molecules (rotate mode, translate mode, scale mode and center, etc.), (g) an easy and efficient choice of underscoring different elements (alpha helices and beta sheets) of the protein secondary structure, (h) users' friendly animation reverses directions, animation tools, types, and controls of the MD and Monte Carlo simulation trajectories, (i) molecule status setting window with (*T*)op molecule, (*A*)ctive, and (*D*)rawn toggles, (j) dynamic graphics (elapsed time, total dipole moment, changing atom properties with color, etc.) adding tools to the trajectory, etc. [37–39]. Despite bestowing all these advanced potential features, not a single disciplinary research work utilizes all of them for the specific purpose. Present author mostly uses the VMD for visualizing the ongoing MD simulation & the time series MD trajectories, for rendering the image of the complex biomolecules, for envisioning the three dimensional model of the polymeric type proton exchange membrane (hereafter, PEM), for displaying the PEM hosted active electrolytes of the redox flow battery technology from the MD simulation derived database, for exhibiting the molecular views associated with the inter-water and electrolyte ion-water radial and angular distribution functions, and for interpreting the molecular models of the active electrolytes lying at the interfacial region of the PEM-electrolyte composites. All the concerned VMD generated splendid visuals and the corresponding snapshots are displayed in Figure 15 to Figure 17 where the precisely mentioned caption describes what the specific images are all about.

(a)

```
ATOM   3141  OW   WAT    5       4.669 -22.166 -36.560
ATOM   3142  HW   WAT    5       5.222 -21.338 -36.560
ATOM   3143  HW   WAT    5       5.222 -22.993 -36.560
ATOM   3144  OW   WAT    5     -44.826 -22.071 -15.281
ATOM   3145  HW   WAT    5     -44.273 -21.243 -15.281
ATOM   3146  HW   WAT    5     -44.273 -22.898 -15.281
ATOM   3147  OW   WAT    5     -17.963   8.238  38.236
ATOM   3148  HW   WAT    5     -17.410   9.066  38.236
ATOM   3149  HW   WAT    5     -17.410   7.411  38.236
```

(b)

```
12   F    1.1731870E+00 -5.3589940E+00 -2.1721040E+00 -0.1649000E+00
13   O    3.0878010E+00 -3.9143310E+00 -8.4997100E-01 -0.2604000E+00
14   C    4.3860740E+00 -4.5432020E+00 -7.4308000E-01  0.3200000E+00
15   F    4.0745430E+00 -5.0117250E+00  5.2681300E-01 -0.1600000E+00
16   F    3.7199320E+00 -5.8344950E+00 -1.2297870E+00 -0.1600000E+00
17   C    5.8860740E+00 -4.8432020E+00 -7.4308000E-01  0.3218000E+00
18   F    6.4745430E+00 -5.0117250E+00  5.2681300E-01 -0.1662000E+00
19   F    5.7199320E+00 -6.0344950E+00 -1.2297870E+00 -0.1662000E+00
20   C    7.2630980E+00 -4.2996550E+00 -1.5682960E+00  0.3216000E+00
21   F    7.6155760E+00 -3.0982070E+00 -1.1201000E+00 -0.3278000E+00
```

Figure 14. A small part of the FORTRAN programming based MD simulator generated VMD readable file formats with (a) *.pdb*, and (b) *.imp* extensions. These type files assessing skill of the VMD actually enables itself to link directly with the MD simulation generated trajectories, time series intermittent geometries, and large material assemblies containing hundreds of millions of atoms and molecules. It is equally compatible with the flexible, editable, extendable, and completely open-source type users' friendly unrestricted features of the MD simulator. It also allows prompt call of the in-built programming scripts for the immediate showing off, interpretation, animation, and analyses of the giant periodic or non-periodic molecular assembly. The MD trajectory files with the *.xyz* extension can also be read *via* the VMD application tool, and visualized the movement of the atoms over the desired picosecond timescale. Beside this, the VMD can be used to assess the temperature and energy files with *.log*/*.dat* extensions produced from the both equilibration and production runs.

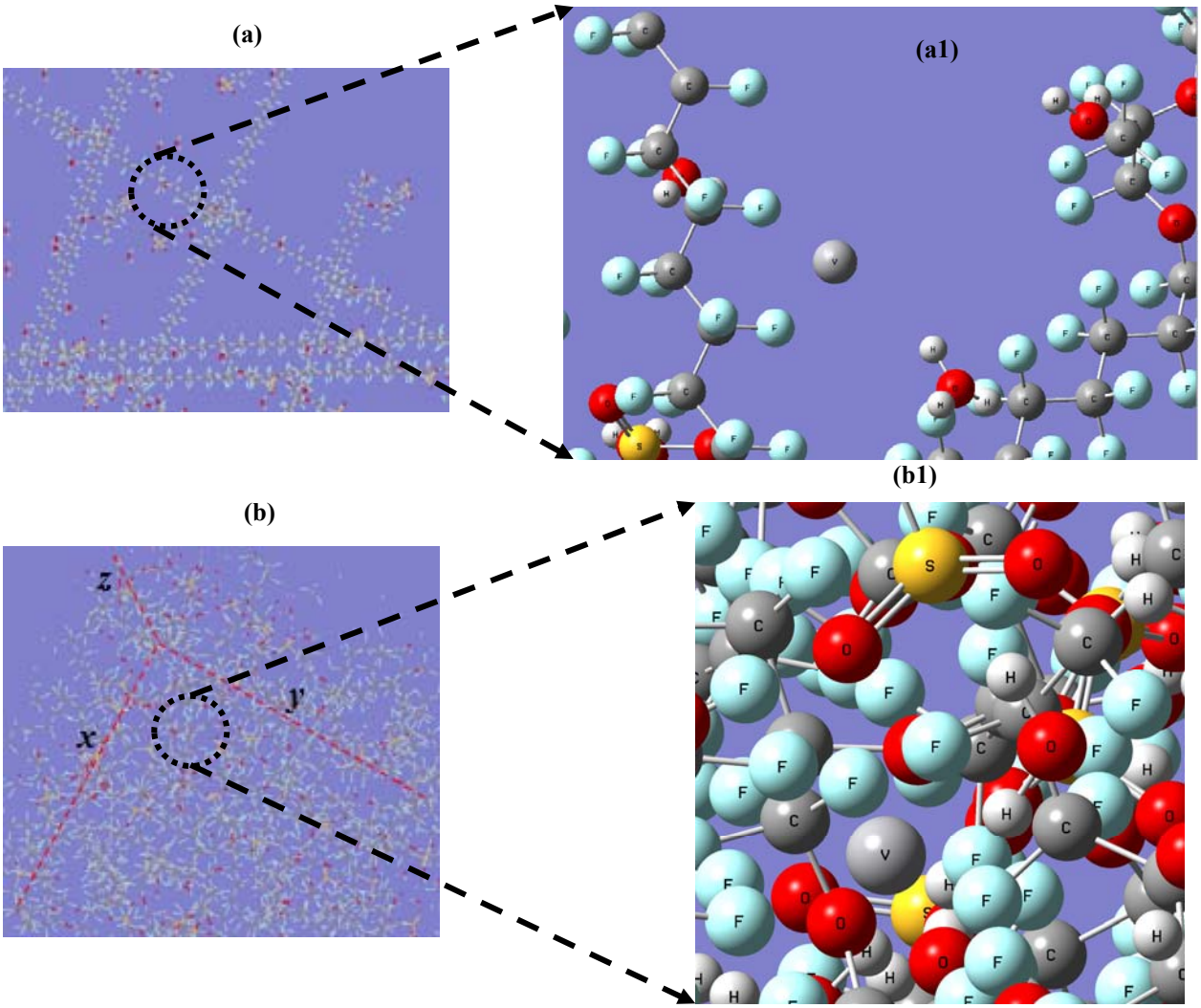


Figure 15. The VMD rendered snapshots of the simulating systems with electrolytic ion and polymeric membrane (**a**) before annealing, (**b**) after annealing. The encircled regions in (**a**) and (**b**) are zoomed out in (**a1**) and (**b1**) respectively in order to get the most possible widest visuals of the scene. This rendering skill of the prompt-called VMD is highly useful not only to examine the initial structure of the simulating systems before running a simulation job, to visualize whether the structure comprises organized arrays of the ions/atoms/molecules/fragments or not, but also to inspect the equilibrium simulations time to time while the simulation jobs and the concerned computational tasks are on the fly. Accordingly, the VMD derived magnificent image is a very trustworthy graphical source to validate the lattice-like structure of the simulation box with confined molecular/ionic structures, fragments, polymeric membranes, etc. (Figure b). More important is to display the views associated with the production simulation trajectories and the time series trajectories for the immediate confirmation of the molecular assembly, and to propose the high-precision evaluations of temperature and pressure for the MD simulations run with a large time step. More especially, a molecular trajectory visualization and editing features of the VMD with options to delete specific frames or set of frames from the animation list can be used to write the Cartesian coordinate sets to the specific files along with rendering graphical images explicitly.

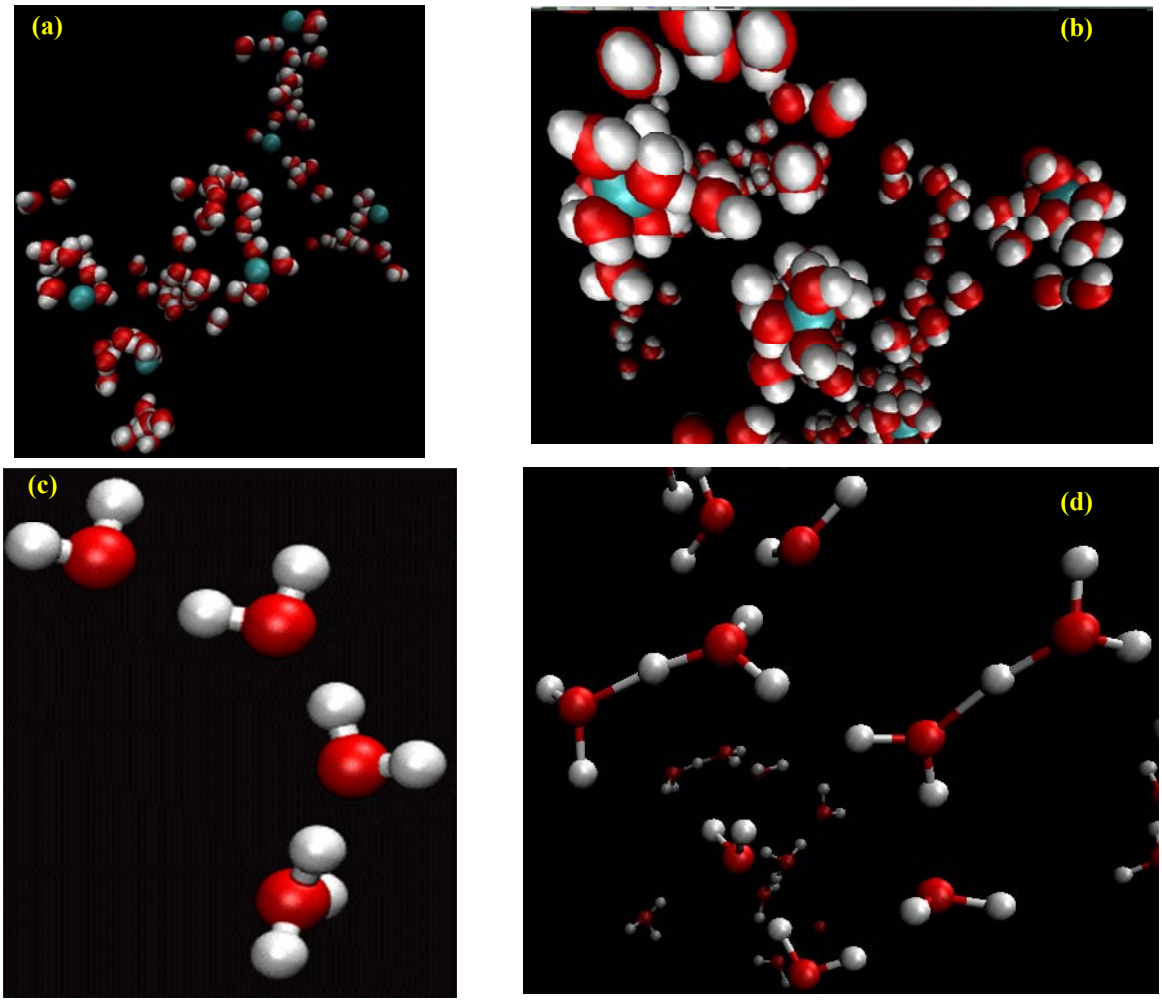


Figure 16. The VMD generated close-up graphical views of the MD simulation trajectories. Such type images are extremely essential to visualize how many atoms/ions/molecules/fragments, etc. fall in the specific regions, to identify the average distribution of the particles around any specific tagged particle within the system, to elucidate the time-averaged density of any constituent particles, to predict the statistical description of the local packing around any reference particles, to determine the distances between each pair of atoms/ions/molecules/fragments, and to approximate how many of such type pair distances lie into that particular sites (radial distribution function RDF $g(r)$). More importantly, the multiple coordination shells and the specific coordination numbers of the each simulating particle can be quantitatively analyzed through this visualization schemes.This quantitative information eventually acts as key parameters for calculating the thermodynamic properties (internal (potential) energy and pressure) of the system. The "Radial Pair Distribution Function $g(r)$" feature of the VMD can be directly employed to calculate the RDF with the explicit molecular visualizations side by side. This feature acts as an invaluable operational tool to understand the arrays of the molecular alignments in the wide ranged liquid systems; to retrieve the live movies of the proton transport mechanisms through Grotthus and vehicular schemes as illustrated in Figure **c** and Figure **d**; to observe the rare crystal defects exist in the crystalline solid; to simplify the regular internal structure of the real gases systems; to estimate the local distribution of ions around the biomolecules such as DNA, to study the protein hydration, and to investigate the dissolution phenomena of the glucose, and its linear polymer glucan, etc.

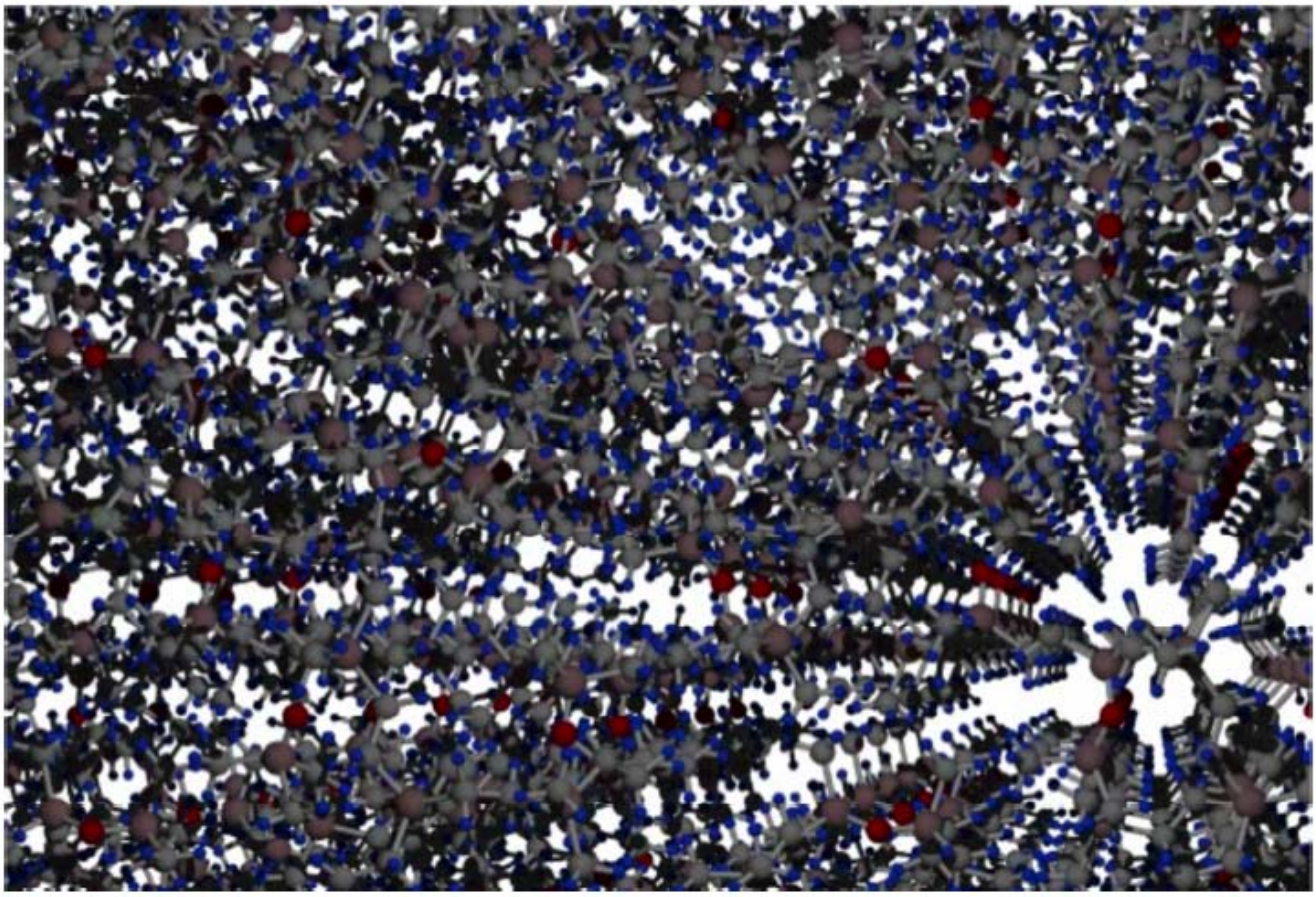


Figure 17. A VMD rendered snapshot of the super cell with siloxaalkane molecular assemblies after 1 ns MD simulation. The periodic boundary condition with the X-ray derived lattice vectors ***a*** = 11.84, 0.000, 0.000; ***b*** = 0.000, 14.619, 0.000; and ***c*** = –3.884, 0.000, 23.874 were used to transform its unit cell to super cell. Usually, visualizing the supercell with hundreds of atoms/molecules/ions in three dimension is quite essential while (a) abstracting the concrete image of the entire solid state crystalline molecular assembly, (b) understanding/interpreting the effect/most probable-locations of the inter-/intra-molecular H-bonding in the molecular network, (c) studying the atomic/molecular closeness, packings, void space, and inter-particle interactions (diagonal, non-diagonal) quantitatively, (d) visualizing the supramolecular ordering/self-organization of the organic molecules, functionalized fullerenes, pentacenes, etc. chemisorbed on the external surface of the crystalline or metallic substrates, (e) investigating the energetics, structure, and dynamics of C60 type molecules on the Au(111), Ag(111), Si(111), Ge(111) surfaces, etc., (f) tracing out the sites of the adsorbent on which adsorbates sit, and their nature of the rotations (clockwise or anticlockwise) with tilt angles for each rotation, (g) confirming the STM generated diversified lattice orientations of the C60, C70 type monolayer structures grown on the solid substrates, (h) performing the total energy calculations of the different systems and evaluating the dependence of formation energies on the cell size, (i) rationalizing the dependency/independency of the defect formation energy with the cell size, (j) quantizing the effect of the dopant on the volume of the supercell, (k) modeling the adsorption stack-assembly of the acids on graphene, etc. surfaces. This specific image is extracted from the paper Ref [40] of the same author.

III. Summary And Conclusion

This short article targeted to the students, chemists, industrial specialists, young research fellows, educators, faculties, academicians, laboratory technicians, etc. mainly describes very fundamentals of the advanced computer graphics aided molecular visualization and manipulation softwares, and chemical & molecular graphics tools & techniques compatible with the quantum chemistry calculation packages. Actually, to the knowledge of this author, many of these academic personalities are constantly suffering from the proper usage and the principal objectives of utilizing such type tools in different scholarly academic and educational endeavors such as teaching and teaching pedagogies; researching and publishing professional activities;

modeling, simulating, and animating purposes of the crystalline or non-crystalline chemical compounds; and visualizing/ interpreting the quantum mechanically derived results with and/or without human unreadable datasets. Beside this, even the expert manpowers are hardly familiar with when, where, and how to apply many freely available chemical graphics based chemistry & chemical education apps, and their fascinating teaching & research tools despite being them the educationally sound and profound molecular graphics designed especially for mimicking the chemistry & chemistry based science experiments and the entire molecular physicochemical properties via the advanced electronic gadgets. With this technical academic attributes, the principal objective of this article was set to lie within the range of triggering all the potential users of the chemical & molecular graphics, and the associated chemistry apps for the utmost utilizations of the later as the most fundamental yet primary tools and techniques in a wide range of complex research fields & teaching philosophies; molecular demonstrations & animations; drug design & discovery; learning, sharing, & publishing scientific information; molecular dynamics & ground state energy calculation strategies; bio- /molecular structural manipulation & interpretation endeavors; pharmacophores identifications techniques; etc., and for the continuous promotion of their incredible constantly-upgrading graphical features to the inclusive scientific education in advancing scientific justice & clarifications, and in underscoring the significance of their decent rendering abilities to the rapid development of chemistry and computer aided chemical researches. In spite of the availability of several advanced electronic gadgets assisted graphical tools, this study most preferentially selected the four topmost suitable yet users' friendly chemical graphics, viz., Molden, GaussView, Jmol, and Visual Molecular Dynamics (VMD) as their representatives, and highlighted the significance of their rendered images with the splendid scenes & visualizations for conceptualizing the chemistry and applied science research & education, and the necessities of manipulating 3D structures of the molecules ranging from small to giant material assemblies for the inherent insights into the chemistry and its complexity.

As per the experiences of the present author, Molden is one of the very customarily used molecular graphics worldwide whose graphical sketches rendering abilities of the molecules and their assemblies in wireframe, ribbon, and Van der Waals modes are quite preferable and referable not only for the instant inspection of the ongoing computational procedures, for the thorough precise monitoring of the constancy of the Gaussian in-built explicit convergence criteria & their graphical variations with the computational steps, for the exact identification of the sites where the specific parts, fragments, and elements have to be placed in order to design/develop a complete prototype molecular model but also for the immediate visualizations & manipulations of the types of atoms, their connections with bonds, angles, & dihedral angles, and the prompt detection of the Gaussian generated Cartesian coordinates of the atoms & their misleading coordinates if any. The Z-matrix editor feature in Molden is very typical and desirable tools as it lets the users building on-screen Z-matrix of the basically small and moderate size molecules conveniently step by step, and facilitating other several aspects of the molecular modeling such as creating, editing, constructing, and manipulating the entire molecular structures and their geometries. Accordingly, the Gaussian, Inc. licensed source codes *GaussView*, possibly the most spectacular, advanced, powerful, and users' friendly computer graphical interface, is also a very frequently used molecular modeling software mainly to execute all the Schrodinger wave mechanical equation based computational/theoretical outputs, human unreadable complex datasets, and the entire molecular wave function based computational procedures. This interface offers exceptional chemical and molecular graphics features compatible with the progressively revised and released Gaussian-series run quantum mechanical calculations & the wave function based numerical derivations, and bestows the most superb molecule-building up techniques side by side because of which it is highly preferable and likeness tools among the theoretical, computational & experimental laboratory instructors, and teaching & research faculties. The molecular orbitals (MOs) editor pop-up window of this software is unique to all the multitask chemistry learners and their multiobjective research problems as it enables them to display magnificent views of the every assigned MOs including HOMO & LUMO with & without electron occupancy, and the corresponding contour diagrams with & without electron cloud along with the explicit presentation/indication of the quantum chemistry derived Eigen values (*E*). Unlike in Molden, this feature extends extraordinary advantages more especially while retrieving the electron density of the MOs and the chemical bonds, total electron density surfaces of the molecules, electrons' amplitudes measuring three dimensional contour plots and lines, MOs iso-surfaces & their explicit contours, alpha electron density surfaces, and the ESP mapping of all the occupied and virtual MOs. As an additional visualization and manipulation tool, the Jmol software, a java-based open-source chemical and molecular graphic codes, is also used frequently by the chemists, educators, researchers, and other molecular modelers due to its distinctive data handling & accessing abilities, and the unique features for modeling crystals, materials & biomolecules. In contrary to both Molden and GaussView, the Jmol can execute almost all type file formats with (a) Cartesian coordinates of the atoms with 'EP' as a dummy, nonexistent atom; (b) MODELLER generated model with 'HETATM' residues on the top and the connected chain of

atoms on the bottom; (c) MOPAC and Molden created Z-matrix datasets, etc., and the various quantum chemistry software package derived computational outputs. The same are the reasons why it is mostly known among the users as a single special type open-source program designed mainly for assessing the relative importance of all these data formats, accessing them efficiently, and displaying the concerned three dimensional molecular models with and without bounding box, crystallographic axes, unit cell dimensions, etc. Beside this, its exceptional measurements, animations & vibrations tools, surface tool, Gaussian input file generator, electron density surface tools with solvent and solvent-accessible regions, and the spectral visualization tools are highly recognizable as they ease computational interpretations, and analyses of the quantum chemistry package revealed theoretical results, and facilitate the users for realizing & exploring the chemistry & its novel aspects. Despite possessing all these potential and prospective features, the Molden, GaussView, & Jmol application tools lack their capabilities of utilizing computational resource platforms and computing technologies, hardware requirements, data storage, CPU timing, computer memory, and the disk storage less. Towards these technicalities, the Visual Molecular Dynamics (VMD) software; a C++ programming code based computationally cheap, cost-effective, and high performance visualizing molecular and chemical graphics tool; is conceded as a quite efficient rendering mean that utilizes relatively limited computational resources, but performs extraordinarily. Additionally, it's unique software designation with special emphasis on the data handling skills and rendering tools for accessing extremely big size molecular dynamics (MD) simulation systems, and their MD & time-series trajectories is awesome. Beside this, the VMD application tools are highly acknowledged due to hosting many more relatively better and advanced potential features such as (a) displaying, manipulating, and visualizing the multiple scenes of the complex molecular systems with the proper indication of the subset of the atoms, (b) multi-formats data files with *.pdb*, *.psf*, *.dat*, *.imp*, *.txt*, etc. extensions and the *dcd* trajectories with no information of the atoms & their connectivity accessing abilities, (c) an easy and efficient choice of underscoring alpha helices, beta sheets, etc. of the protein secondary structure, (d) users' friendly animation reverses directions, animation tools, types, and controls of the MD and Monte Carlo simulations, etc. Moreover, this software is more particularly known among the users as a "Radial Pair Distribution Function (RDF) $g(r)$" hosting tool which can be employed directly in determining the RDF values efficiently and systematically with the explicit molecular visualizations side by side. This feature is very invaluable operational graphical tool while expressing theoretical insights into the arrays of the molecular alignments in the wide range liquid/fluid systems, the rare crystal defects existing in the crystalline solid state systems, the regular internal structure of the real gases systems, the local distribution of ions around the biomolecules such as DNA, the protein hydration & the dissolution phenomena of the glucose and its linear polymer glucan, etc.

In view of all the aforementioned applications features of the advanced electronic gadgets assisted molecular & chemical graphical tools and their groundbreaking performances, each and every molecular building, visualizing, & manipulating software deserves big round of applause and remarkable appreciations. Even though not a single discipline of the science and the cutting-edge research utilizes all the available features bestowed by each and every graphical softwares, their similar style graphical prominent offers; unique modeling & manipulating principles; and the overall philosophy of searching/studying three dimensional molecular structures/geometries & their typical physicochemical properties make themselves quite fundamental yet indispensable means of conceptualizing chemistry and chemical education.

NOTE

The author declares no competing financial and non-financial interests.

ACKNOWLEDGEMENT

This scholarly research work is carried out under the affiliation of Kathford International Education & Research Foundation, Lalitpur, Nepal. The author is indebted to Dr. Indira Kadel, Senior Divisional Meteorologist at Department of Hydrology and Meteorology, Ministry of Energy, Government of Nepal for her fruitful discussions on potential applications of computer graphics in climate science & weather forecasting. The editorial and reviewer board members are acknowledged for their constructive reviews.

REFERENCES

[1] D. J. Eck, W. Smith, Introduction to Computer Graphics (David J. Eck, 2016).

[2] S. Marschner, P. Shirley, Fundamentals of Computer Graphics: International Student Edition (A K Peters/CRC Press, 2021).

[3] G. Ciccotti, C. Dellago, M. Ferrario, E. R. Hernandez, M. E. Tuckerman, Molecular simulations: past, present, and future (a Topical Issue in EPJB), *The European Physical Journal B*, Vol. 95, No. 3, pp 1–12, 2022.

[4] A. Hospital, JR O. M. Goni, J. Gelpi, Molecular dynamics simulations: advances and applications, *Advances and Applications in Bioinformatics and Chemistry*, Vol. 8, pp. 37–47, 2015.

[5] W. T. Wipke, Evolution of Molecular Graphics, (American Chemical Society, 1987).

[6] K. I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, (Springer-Verlag Berlin Heidelberg, 2008).

[7] C. E. Sansom, C. A. Smith, Computer applications in the biomolecular sciences. Part 1: molecular modelling, *Biochemical Education*, Vol. 26, pp. 103–110, 1998.

[8] C. Liao, M. Sitzmann, A. Pugliese, M. C Nicklaus, Software and resources for computational medicinal chemistry, *Future Medicinal Chemistry*, Vol. 3, Issue 8, pp.1057–1085, 2011.

[9] B. G. Levi, Nobel Prize Honors Kohn and Pople for Methods of Quantum Chemistry, *Physics Today*, Vol. 51, Issue 12, pp. 20–22, 1998.

[10] A. B. Marahatta, A DFT Analysis for the Electronic Structure, Mulliken Charges Distribution and Frontier Molecular Orbitals of Monolayer Graphene Sheet, *International Journal of Progressive Sciences and Technologies*, Vol. 16, No. 1, pp. 51–65, 2019.

[11] A. B. Marahatta, Effect of *n*-Type Dopant Nitrogen in the Structure and Atomic Charges Distribution of Monolayer Graphene Sheet: A DFT Analysis, *International Journal of Progressive Sciences and Technologies*, Vol. 16, No. 2, pp. 01–13, 2019.

[12] M. J. R. Yunta, Using Molecular Modelling to Study Interactions between Molecules with Biological Activity, (Bioinformatics, 2012).

[13] M. Aminpour, C. Montemagno, J. A. Tuszynski, An Overview of Molecular Modeling for Drug Discovery with Specific Illustrative Examples of Applications, *Molecules*, Vol. 24, No. 1693, pp. 1–30, 2019.

[14] A. B. Marahatta, Computational Study on Electronic Structure, Atomic Charges Distribution and Frontier Molecular Orbitals of Butadiene: General Features for Diels-Alder Reaction, *International Journal of Progressive Sciences and Technologies*, Vol. 19, No. 2, pp. 48–64, 2020.

[15] A. B. Marahatta, The QSPR Studies of [SO4 (H2O)n]2−, *n* = 1-4, 16 Clusters through Quantum-Chemical Descriptors, *International Journal of Progressive Sciences and Technologies*, Vol. 27, No. 2, pp.441–454, 2021.

[16] A. B. Marahatta, Energy, Electronic, and Reactivity Descriptors in Quantitative Structure Property Relationships of [HSO4(H2O)*n*]−, *n* = 0, 3, 4, *Chemistry Research Journal*, Vol. 7, Issue 2, pp. 56–69, 2022.

[17] A. B. Marahatta, DFT Study on Electronic Charge Distribution and Quantum−Chemical Descriptors for the Kinetic Stability of Vanadium Aquo Complex Ions [V(H2O)6]2+ and [V(H2O)6]3+, *International Journal of Progressive Sciences and Technologies*, Vol. 22, No. 1, pp. 67–81, 2020.

[18] A. B. Marahatta, Relative Kinetic Stability Study of Hydronium, Zundel, and Eigen Cations through Quantum Mechanical Molecular Orbitals Approach, *International Journal of Progressive Sciences and Technologies*, Vol. 23, No. 1, pp. 473–486, 2020.

[19] M. Aminpour, C. Montemagno, J. A. Tuszynski, An Overview of Molecular Modeling for Drug Discovery with Specific Illustrative Examples of Applications, *Molecules*, Vol. 24, Issue 1693, pp. 1–30, 2019.

[20] M. Luo, O. A. Mazyar, Q. Zhu, M. W. Vaughn, W. L Hase, L. L. Dai, Molecular dynamics simulation of nanoparticle self-assembly at a liquid-liquid interface, *Langmuir*, Vol. 22, Issue 14, pp. 6385−6390, 2006.

[21] A. B. Marahatta, M. Kanno, K. Hoki, W. Setaka, S. Irle, H. Kono, Theoretical Investigation of the Structures and Dynamics of Crystalline Molecular Gyroscopes, *Journal of Physical Chemistry C*, Vol. 116, pp. 24845−24854, 2012.

[22] D. Horinek, J. Michl, Surface-mounted altitudinal molecular rotors in alternating electric field: Single-molecule parametric oscillator molecular dynamics, *PNAS*, Vol. 102, Issue 40, pp. 14175−14180, 2005.

[23] J. Vacek, J. Michl, Artificial Surface-Mounted Molecular Rotors: Molecular Dynamics Simulations, *Advanced Functional Materials*, Vol. 17, Issue 5, pp. 730−739, 2007.

[24] S. Lehtola, A. J. Karttunen, Free and open source software for computational chemistry education, *WIREs Computational Molecular Science*, Vol. 12, Issue 1610, pp. 1–33, 2022.

[25] G. Schaftenaar, J. H. Noordik, Molden: a pre- and post- processing program for molecular and electronic structures, *Journal of Computer-Aided Molecular Design*, Vol. 14, pp.123–134, 2000.

[26] W. J. Hehre, W. A. Lathan, R. Ditchfield, M. D. Newton, J. A. Pople, Gaussian 70 (Quantum Chemistry Program Exchange, Program No. 237, 1970).

[27] Expanding the limits of computational chemistry (Gaussian Inc., 2015); *https://gaussian.com/*.

[28] C. Breno R. dos Santos, C. C. Lobato, M. A. Costa de Sousa, W. J. da Cruz Macêdo, J. C. T. Carvalho, Molecular Modeling: Origin, Fundamental Concepts and Applications Using Structure-Activity Relationship and Quantitative Structure-Activity Relationship, *Reviews in Theoretical Science*, Vol. 2, pp. 1–25, 2014.

[29] A. B. Marahatta, Effect of *n*-Type Dopant Nitrogen in the Structure and Atomic Charges Distribution of Monolayer Graphene Sheet: A DFT Analysis, *International Journal of Progressive Sciences and Technologies*, Vol. 16, No. 2, pp. 01–13, 2019.

[30] A. B. Marahatta, A DFT Study of Electronic Structures on Hydrated Sulfate Clusters [SO42−(H2O)*n*] *n* = 0−4, 16, *International Journal of Progressive Sciences and Technologies*, Vol. 17, No. 1, pp. 55–69, 2019.

[31] M. Yagmurcukardes, S. Horzum, E. Torun, F. M. Peeters, R. T. Senger, Nitrogenated, phosphorated and arsenicated monolayer holey graphenes, *Physical Chemistry Chemical Physics*, Vol. 18, pp. 3144–3150, 2016.

[32] Jmol: an open-source Java viewer for chemical structures in 3D. *https://jmol. sourceforge.net/.*

[33] X. J. Chen, Guide to Graphics Software Tools, pp. 471, (Springer, 2008).

[34] A. Herráez, Biomolecules in the Computer: Jmol to the Rescue, *Biochemistry and Molecular Biology Education*, Vol. 34, Issue 4, pp. 255–261, 2006.

[35] A. Herráez, How to Use Jmol to Study and Present Molecular Structures, Vol. 1, pp. 21, (Lulu.com, 2008).

[36] A. B. Marahatta, H. Kono, SCC-DFTB Study for the Structural Analysis of Crystalline Molecular Compasses, *Chemistry Research Journal*, Vol. 7, Issue 4, pp. 77–94, 2022.

[37] W. Humphrey, A. Dalke, K. Schulten, VMD: Visual Molecular Dynamics, *Journal of Molecular Graphics*, Vol.14, pp. 33−38, 1996.

[38] VMD user's guide (version 1.9.3), 2016. *https://www.ks.uiuc.edu/Research/vmd /current/ug/*

[39] R. Johnson, Visual Molecular Dynamics User Guide, *https://www.sas.upenn.edu/~robertjo/ html-physics/vmd/VMD%20User%20Guide.pdf*

[40] A. B. Marahatta, Geometry Optimization Skills of DFTB: Simple to Complex Molecular Systems, *International Journal of Progressive Sciences and Technologies*, Vol. 15, No. 2, pp. 263–277, 2019.