An Easy-to-Use Three-Dimensional Molecular Visualization and Analysis Program: POSMOL

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Received June 10, 2004

Molecular visualization software has the common objective of manipulation and interpretation of data from numerical simulations. They visualize many complicated molecular structures with personal computer and workstation, to help analyze a large quantity of data produced by various computational methods. However, users are often discouraged from using these tools for visualization and analysis due to the difficult and complicated user interface. In this regard, we have developed an easy-to-use three-dimensional molecular visualization and analysis program named POSMOL. This has been developed on the Microsoft Windows platform for the easy and convenient user environment, as a compact program which reads outputs from various computational chemistry software without editing or changing data. The program animates vibration modes which are needed for locating minima and transition states in computational chemistry, draws two and three dimensional (2D and 3D) views of molecular orbitals (including their atomic orbital components and these partial sums) together with molecular systems, measures various geometrical parameters, and edits molecules and molecular structures.

Key Words : Molecular program package, Molecular visualization, Molecular graphics, Molecular orbital density, Normal mode

Introduction

The use of computer graphics for visualizing outputs of scientific and engineering software has been rapidly spread for the recent years.[1] The molecular visualization software has received high recognition in a wide variety of fields such as chemistry, biochemistry, physics, biology, fluid dynamics, computer aided drug design, etc. These types of specialized software have accelerated the scientific innovation, since most data can be analyzed in a more concrete way. The continuous development of visualization and analysis programs makes it possible for users to visualize many complicated molecular structures on personal computers and workstations. However, users are often discouraged from using these tools due to the difficult concept or complicated user interface.

Some of the essential requirements of good visualization software are (i) efficiency, (ii) user-friendliness, (iii) seamless human-machine interface, etc. Taking these requirements into account, we have developed an extremely efficient and versatile visualization and analysis software, POSMOL, which is the acronym for Postech (Pohang University of Science and Technology) Molecular Program Package. Apart from fulfilling all the requirements of a good visualization and analysis software, POSMOL enables one to carry out a wide range of graphical tasks as an effective graphical front-end to various computational chemistry software. Molecular images by POSMOL have been used in various publications.[2,3] The initial package development for POSMOL started in 1987 to visualize the dynamical changes of molecular structures for the generalized molecular dynamics analysis (GMDA) program package which was developed during 1985-1987 (unpublished) and used in biomolecular dynamics studies.[4] This initial program which focused on the structural analysis, has been enforced by adding photorealistic image generation using the ray-tracing technique.[5] Then, it was completely revamped[6] by using the graphics library, OpenGL,[7] and has been revised recently.

The POSMOL simplifies its use by removing some intricate interface and customizing graphical interface. The choice of the molecular visualization tool may be a matter of user's preference. However, strong factors in the choice may also be influenced by compatibility with the format of users data set, output options, connection with many simulation codes, chemistry calculation programs, and options for visual representation of data. Our research group needed to have a new molecular visualization software that is specific to our particular requirement. The development of POSMOL was motivated by such a need. Visualization of computational results is an important process for analysis and interpretation. POSMOL has been designed as a visualization tool to analyze the results of computational chemistry programs, such as GAUSSIAN, GAMESS, Q-CHEM, ACES, AMBER, and CHARMM which have become widely available and accepted as valuable tools in computational chemistry.[8] The program has focused on displaying easy-to-

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use editable three-dimensional molecular structures and generating high quality images. For the visualization of calculated results, we opted to use a widely available graphics library, OpenGL.[8] OpenGL allows real-time manipulation of three-dimensional objects with relatively small instructions which consist of approximately 120 distinct commands. OpenGL is designed as a streamlined, hardware-independent interface which can be implemented on many different platforms. It is able to build up models of complicated three-dimensional objects from simple geometric primitives such as points, lines, polygons, images and bitmaps. This simple and easy-to-use graphics library allows users to create interactive programs that produce and edit various color images of three dimensional molecular motion.

Program Features

POSMOL has the following features:

• The program can draw, render, edit, and analyze 3D molecular structures fast even on low-performance personal computers.

• The output files of computational chemistry programs, such as GAUSSIAN, GAMESS, Q-CHEM, ACES, AMBER, and CHARMM can be directly loaded to POSMOL to obtain high quality 3D images of various molecular conformations and molecular orbitals. POSMOL can read the Protein Data Bank (PDB) format and Cambridge structural data base.

• The program is very compact. Effective algorithms and graphics Application Program Interface (API) which help rapidly draw molecular images are implemented in the program.

• The program can generate schematic normal modes from the result of vibrational frequency calculation. It can also animate normal modes. It allows the user to find the trajectory toward the minimum energy state and transition state from the frequency analysis of quantum chemical programs, and monitor dynamic trajectory from molecular dynamics simulations.

• The program generates high quality images. The Device Context attached to the personal computer is directly used instead of printing rendered images for the full resolution of the attached printer.

• POSMOL can draw 2D and 3D molecular orbitals regardless of basis sets used in computational programs using molecular orbital coefficients and basis set information. Molecular orbitals (including the atomic orbital components and their partial sum) along with molecular structures can be translated, rotated, zoomed, edited, and printed.

POSMOL has been primarily developed to provide a direct visualization of the calculation results obtained from computational chemistry programs. For the convenient user environment, we have chosen Microsoft Windows platform. POSMOL has been written on Microsoft Windows NT using Visual C++ version, Microsoft Foundation Class (MFC) and OpenGL API. POSMOL also runs on the Windows NT and XP. POSMOL is coded with highly optimized and effective algorithms. Therefore, it shows very good performance. Since OpenGL can be applied to a number of platforms, including SGI, SUN, HP, etc. with very similar function, its core functionality can be easily ported to other platform.

POSMOL and OpenGL

OpenGL has recently become the most widely used 2D and 3D graphics API. OpenGL has been developed as a low level interface to their proprietary graphics hardware. OpenGL is controlled by an independent consortium and is distributed in many operating systems. OpenGL guarantees that the end result will be identical, regardless of the OS platform on which it is running. In POSMOL, we define the geometry of molecules for display, along with the desired rotations, translations, and scaling through function calls to the OpenGL API. OpenGL handles the remaining matrix manipulations, projections, and rendering necessary to place the atoms and bonds on the screen. During visualization, we need to know the geometry of molecules at the beginning and how they should appear on the screen at the end, while we do not need to know anything about the steps which are performed in between. OpenGL allows us to concentrate on implementation of various operations in an optimized way.

Display Effects. The Built-in OpenGL commands provide and control all display effects in POSMOL. The programmer can easily enable or disable the desired effect on a molecular scene with appropriate parameters. In POSMOL, there are several options for display effect supplied by glEnable() function and its modes. These options can be controlled in the preference window. The Point-and-Line option provides a rendering function, which can smooth lines, curves, and surfaces to improve molecular rendering quality. For example, users can choose one from Fast, Smooth, and Anti-aliasing. These functions are represented by enabling or disabling OpenGL attributes such as GL_POINT_SMOOTH, GL_LINE_SMOOTH, and GL_BLEND. If the user selects anti-aliasing function which is a technique for reducing the jagged effect created on molecular wireframe, all three modes are enabled. Dither option is used to present atoms or bonds with limited colors by placing different-colored pixels together in patterns that give the illusion of shading between colors. This option can reduce color data in molecules. The Depth-cue option gives 3D perspective on molecular system. Atoms and bonds away from the eye are dim, just as they would be in a real scene. The Light option allows the user to specify one or more light sources and define their lighting characteristics in terms of AMBIENT, DIFFUSE, SPECULAR and POSITION. The AMBIENT, DIFFUSE and SPECULAR lighting attributes are defined with single RGBA value that describes the relative intensities of red, green, and blue lights and the alpha value that is the fourth color added to provide a degree of transparency to the color of the object. Four elements in POSITION specify the position of the light source.

Drawing Molecules. POSMOL primarily presents three

rendering styles: Wireframe, Circle & Rod and Ball & Stick. Atoms can be drawn in one of the following: dot, circle, disk, and sphere. The atoms can be easily edited. Chemical bonds, H-bonds, and weak bonds can be represented by line, dotted line, 2D rod, pseudo rod, cylinder, and multiple cylinders, and edited. Initially all objects are displayed as wire frames, and there are options for the user to change the value in order to get the desired representation. By selecting the editor in the atom item, the user can modify the radius and color of all atoms or selected atoms. It can create almost all of above three dimensional molecular components using GL functions and GLU quadric routines that enable to draw various 3D objects.

Program Overview

POSMOL consists of menus including icons on the top, a transform toolbar on the left side and multiple work windows on the center of program window. While working with POSMOL, users can manipulate multiple windows, which enable the comparison of different molecules or conformation of the same molecule in different angles. A representative snapshot of POSMOLs working windows is shown in Figure 1.

Input and Output. POSMOL reads the output file from many computational programs and PDB, XYZ, Gaussian formatted checkpoint files, etc. Multiple molecules can be represented and manipulated in a window by importing any number of molecules. It is helpful for superimposing multiple molecules to identify geometrical differences between them. POSMOL can read molecular coordinates and other information from compressed files without decompressing them. POSMOL offers so-called object persistency. It can save the current status to a file and restore it from the file as it is required.

Transformation of objects. POSMOL can perform basic transformations of the objects such as translation, rotation and scaling. It can also align objects along any axis or plane. Two reference objects (usually atoms or dummy points) are used to align objects to an axis, and three objects are used to align them to a plane. There are two types of projection method, Orthographic and Perspective. In the orthographic projection, all objects that have the same dimension are represented with the same size regardless of whether they are away or nearby. In the perspective projection, a distant object is represented smaller than the nearby one. In this case, the user can configure the view angle manually or automatically which affects the relative sizes of far and near objects.

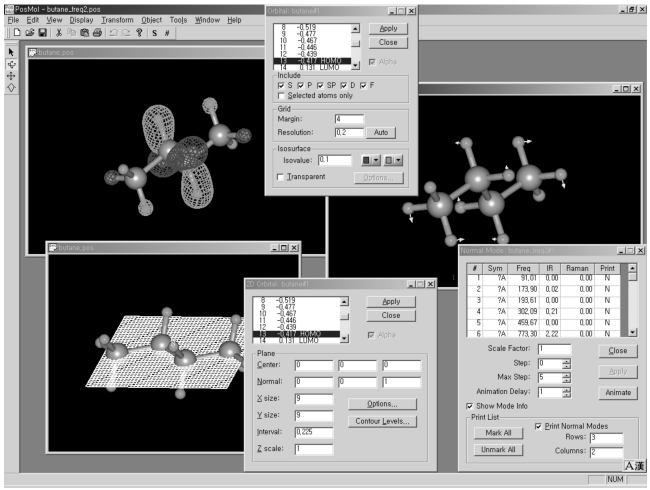

Figure 1. A snapshot of POSMOL desktop.

Analysis Tools

Measure. We can perform the basic measurements such as the XYZ coordinates of an object, the distance between two objects, the angle between three objects, and the dihedral angle between four objects. The object point can be not only an atom position but also a ghost atom position which can be generated as a center of multiple points (*i.e.*, a midpoint between two points, a center a triangular, tetragonal, pentagonal or hexagonal rings). POSMOL offers just one dialog box for these measurements for simplicity and effectiveness of a lot of contiguous operations.

Normal modes. Molecules are often characterized by their spectroscopic properties. IR and Raman spectra are the commonly used spectroscopic methods to identify a molecule. A spectrum can be characterized by a set of intensities and frequencies for the normal modes of vibration. The outputs of computational chemistry programs can now provide the vectors that characterize the displacement of each atom in a particular vibrational mode. Using POSMOL we can perform the static representation and the animation of each normal mode. In the static representation of each normal mode, the molecule is presented as a static object and each displacement of the atoms in the molecule are depicted by an arrow. We can print 3*n*-6 (3*n*-5 for linear molecules) normal modes of

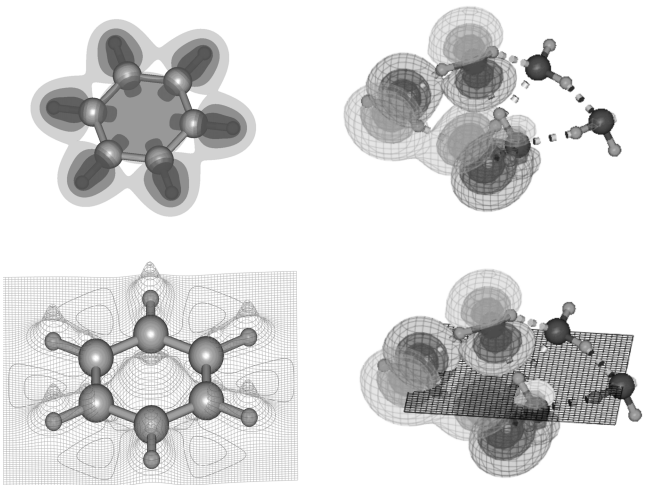

Figure 2. Contour-mesh plot and isodensity surface plot for molecular orbitals of the benzene (left) and the water hexamer (right). Contours can be drawn on the mesh surface in 3D (top) and on a predefined plane in 2D (bottom). Each isosurface is transparently displayed to describe two or three levels of isodensity.

the molecule specifying the options for the number of rows and columns in a page. We can also animate each normal mode. We obtain the relative displacement of atoms in a molecule. Applying these relative displacements of atoms positively and negatively, we can animate each normal mode of a molecule. This can provide the reaction pathway toward a transition state or a local minimum.

Molecular Obital Density. POSMOL can display and manipulate any calculated molecular orbital or total electron density in 2D or 3D graphics space regardless of basis sets. In order to investigate a chemical reaction, it is important to understand the properties of electron distributions. POSMOL generates grid values of an orbital and displays them as an iso-contour level. POSMOL can read the molecular orbital and electron density from a wavefunction. The input file for the orbital or electron density has to include explicit information provided by the quantum chemical programs concerning the details of the basis set and molecular orbitals for the molecule. Two examples of molecular orbital plots of the benzene and the water hexamer[9] are shown in Figure 2.

Concluding Remarks

The present account details the development of a versatile Windows based molecular graphics program (POSMOL) based on OpenGL technology. Apart from several interesting features which are of interest to chemists, the object oriented programming concept used in the development of POSMOL enables easy addition and extension of its capabilities. It can draw molecular orbital densities along with the molecular structures in 2D and 3D spaces, with interactive translation, rotation, scaling, and editing. POSMOL is a molecular visualization and analysis tool which is faster in speed and smaller in size. POSMOL has been used successfully in geometry optimization, normal mode analysis, and molecular orbital analysis. In particular, utilizing the frequency analysis, it has been very useful to locate the minimum and transition states of molecular systems.

Acknowledgment. This research was supported by KOSEF(CRI) and partly by BK21.

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