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REGULAR ARTICLE

Towards interactive 3D graphics in chemistry publications

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Abstract In this paper, we describe how it is possible to extend the visualization and publishing capabilities of the ubiquitous Adobe portable document format (PDF) from the static 2-dimensional (2D) pictures to interactive 3-dimensional (3D) models, 3D-PDF. Embedding 3D scenes of molecules and molecular properties into the electronic Computational Chemistry publications could be very important for visualization of complex molecular properties. No additional 3D-rendering software is required, because the 3D information has been already integrated within the PDF document, which can be displayed by any computer with up-to-date Adobe Acrobat software installed. We briefly describe a computer program, Jamberoo, which can be used for creating 3D-PDF documents and demonstrate several simple examples of integrated 3D models within the PDF. Finally, we show some possibilities of Acrobat JavaScript programming for creating dynamic 3D-PDF content with the elements of the Graphical User Interface (GUI).

Keywords 3D-PDF · GUI · VRML · JavaScript · Visualization · Jamberoo

Dedicated to professor Sandor Suhai on the occasion of his 65th birthday and published as part of the Suhai Festschrift Issue.

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1 Introduction

Computational chemists deal with molecular structures and many molecular properties, for example, molecular surfaces, isosurfaces for molecular orbitals, electrostatic potential, electron densities, etc. which are intrinsically 3-dimensional (3D). There are plenty of molecular-visualization programs, both freeware and commercial ones, which can provide interactive representations of molecular geometry and 3D properties. However, when it comes to the publication of calculated results, visualization is limited to the static 2-dimensional (2D) images, thus limiting effective communication between the authors and readers. Although many scientific publishers allow linking of supplementary materials to the original articles, it could require readers to have dedicated visualization software and tools.

The use of publishing technology which embeds the 3D information into the original paper offers a solution to this problem. This information can then be accessed by all readers interactively without the need for any additional software.

2 Embedding 3D scenes into Adobe PDF

The ubiquitous portable document format (PDF) developed by Adobe Systems Incorporated [1] is currently the de facto standard of scientific publishing. Starting from the Adobe Acrobat 7.0 family in 2005 it has become possible to embed, view, and navigate 3D content in PDF files.

The embedded 3D content can be viewed and manipulated with the free Adobe Acrobat Reader, with no additional visualization software required. Acrobat Reader includes a full set of navigation tools that lets viewers

selectively control the visibility of the model geometry, move to predefined viewing locations, and adjust display modes. The embedded 3D imagery within the PDF documents was successfully demonstrated recently in Astronomy [2] and Chemistry [3] papers.

Kumar et al. [3] described how to embed an interactive 3D content into a PDF document using the PyMOL [4] and Adobe Acrobat 3D Toolkit. In this manuscript, we show how to enhance 3D PDF content with the JavaScript programming and the elements of the GUI such as buttons, checkboxes, combo boxes, etc. Also, at the time of writing of this paper, Adobe released Acrobat Version 9 Pro Extended which incorporates the Acrobat 3D Toolkit, so all our 3D PDF examples and related on-line tutorials are prepared with the Acrobat 9 Pro Extended.

Embedding 3D images into a PDF document can be done relatively easily using Adobe Acrobat 9 Pro Extended which can either convert virtually any computer-aided design (CAD) files (27 CAD file formats are supported) into a PDF document or capture a 3D model from any 3D CAD application that supports OpenGL (standard graphics language for 3D models). The 3D capture is not that straightforward and requires specific settings for different applications in order to work, so we chose the former approach and save each molecular scene in the Virtual Reality Modeling Language (VRML) format [5, 6]. The advantage of the VRML is that it is an ASCII (text) file format which can be visualized by VRML viewers and can be edited in text or VRML editors, i.e., the VRML format gives more control over the 3D scene for advanced users.

To generate 3D scenes in VRML format, we used Jamberoo [7]. Jamberoo is an open-source program for displaying, analyzing, and editing molecular systems, developed at the Supercomputer Facility at the Australian National University. The program can be used for visualizing input and output files for the most popular chemical file formats, ADF [8], Amber [9], Gamess [10], Gaussian [11], Mopac [12], Q-Chem [13], VASP [14], etc. as well as for analyzing volumetric data (molecular orbitals, electrostatic potential, electron densities, etc.) and molecular frequencies.

Jamberoo uses the java3d application programming interface (API) [15, 16] for high-performance 3D graphics. In Java3d, a collection of objects to be rendered forms hierarchical tree structures or scene graphs. A program module for Jamberoo has been developed which takes a Java3d scene graph as input, explores the scene graph path and produces a nearly equivalent VRML graph with the same geometric shapes (spheres, cylinders, surfaces, etc.), geometric transformations, and appearance properties (colors, material attributes, lighting, etc.). The final VRML file containing the molecular 3D scene can be imported into the Adobe Acrobat 9 Pro Extended for editing and subsequent generation of a PDF document with integrated 3D graphics.

If Microsoft Office 2003 or 2007 products (Word, PowerPoint, and Excel) are installed on the user's computer, the Adobe Acrobat 9 Pro Extended will add an additional icon to the PDFMaker toolbar (Office 2003) or the Acrobat ribbon (Office 2007). The Insert Acrobat 3D Model button (Office 2003) and the Embed 3D (Office 2007) button enable a user to insert a preview of a 3D file into the Office document. In Microsoft Office applications, user can adjust the placement, background color, and other properties of inserted 3D models (hide or isolate parts, create new views, and set model perspective). The resulting Office document with the embedded 3D model(s) can be converted into the 3D PDF.

There are several simple examples to illustrate the application of 3D PDF. The first example (Fig. 1) shows a 3D model of the tetrahedrane molecule. A 3D model initially appears as a 2D preview image. To activate the 3D view, click the 2D picture with the Hand or Select tool. The 3D toolbar will appear in the area above the upper-left corner of the 3D model. You can use the 3D toolbar to zoom in and out, rotate, and pan across the object. The Model Tree is used to hide or isolate parts, or make parts transparent.

Figure 2 shows the highest occupied molecular orbital (HOMO) of the C_6F_4 molecule using the Gaussian 03 [11] HF/6-31G* calculation. This example also illustrates another important feature of the PDF-integrated 3D

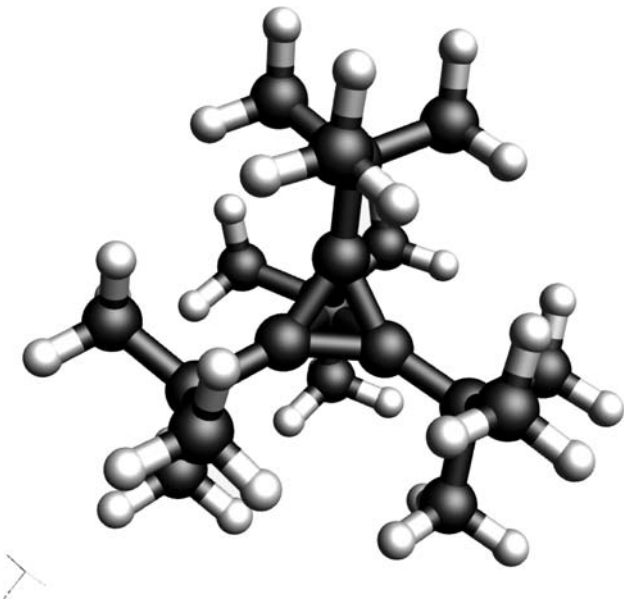

Fig. 1 Interactive 3D model of a tetrahedrane. Click the picture with the Hand or Select tool to activate the 3D model. Use the 3D toolbar to zoom in and out, rotate, and pan across the object. Use the Model Tree to hide or isolate parts, or make parts transparent

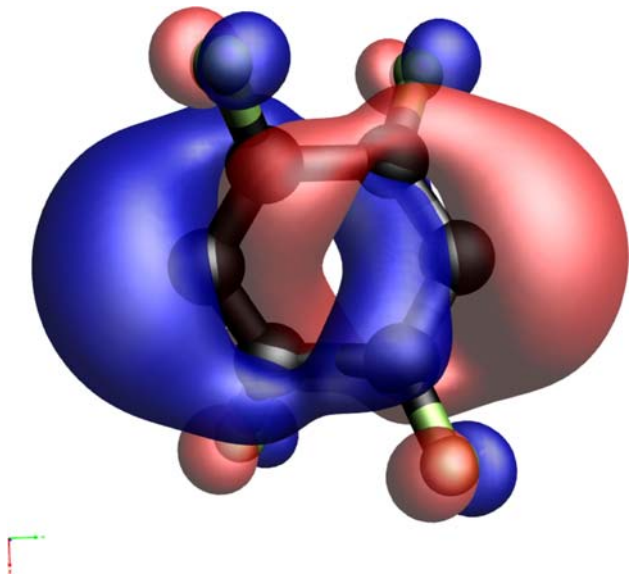

Fig. 2 HOMO of the C_6F_4 molecule. HF/6-31G calculations using Gaussian 03 [11]. Isovalues are 0.02 (*red*) and −0.02 (*blue*). Both isosurfaces consist of ca. 45 thousand triangles. Click the picture with the Hand or Select tool to activate the 3D model

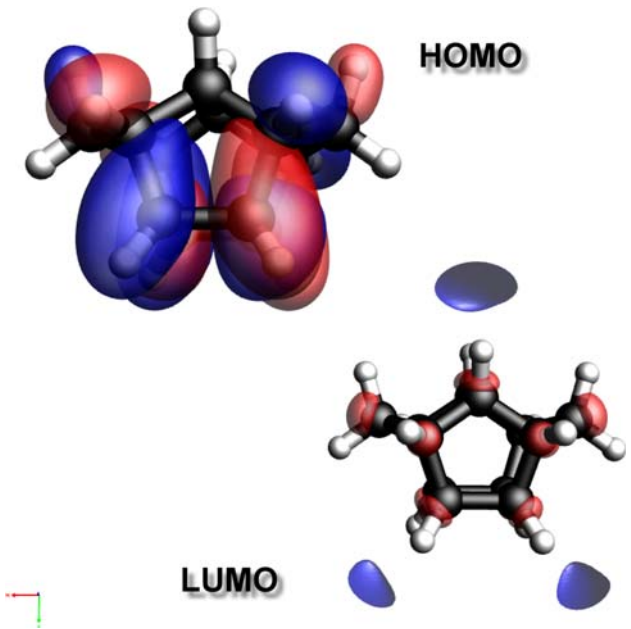

Fig. 3 HOMO and LUMO of a birdcage molecule. HF/6-31G calculations using Gaussian 03 [11]. Isovalues are 0.02 (*red*) and −0.02 (*blue*). Click the picture to activate the 3D model. Use the radio buttons to toggle between HOMO and LUMO

models; custom 3D views. After activation of the 3D model, the list of all available views for the 3D model appears in the Views menu on the 3D toolbar and in the View pane of the Model Tree. Views help readers to navigate quickly the 3D content (such as top, bottom, left, right, inside, outside, etc.).

The author can create additional views of the 3D model in Adobe Acrobat to bring the reader's attention to particular features of a molecular model. A view can include lighting, camera position, rendering mode, the Model Tree state, and transparency and cross-section settings.

3 Embedding the dynamic 3D content into Adobe PDF

Adobe Acrobat can provide far more capabilities than a simple document viewer. It is possible to enhance a PDF document so that it can contain elements of the GUI such as buttons, checkboxes, combo boxes, etc., to initiate user actions. This can be achieved using the Acrobat JavaScript, an object-oriented scripting language developed by Netscape Communications. Acrobat JavaScript implements extensions to the JavaScript language which enable a developer to manage the Acrobat-specific objects.

Figure 3 illustrates the use of the radio button GUI controls to toggle the display of either the HOMO or the lowest unoccupied molecular orbital (LUMO). Acrobat monitors selection of the radio button by reader and executes the appropriate JavaScript code.

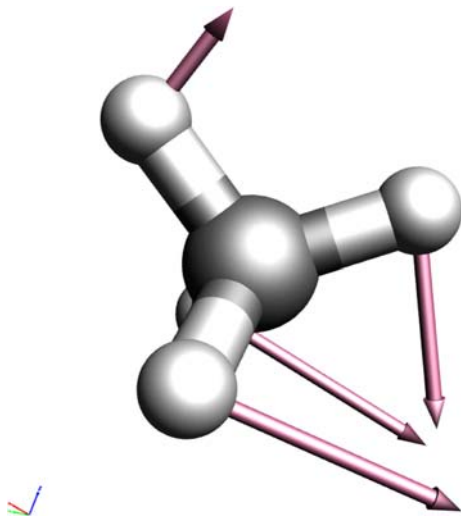

Fig. 4 One of the vibration modes of a methane molecule. Click the picture to activate the 3D model. Click check box to show/hide displacement vectors associated with a given vibration. Buttons "Animate" and "Stop" control the display of animation corresponding to the selected vibration. The molecule can be rotated and zoomed during the animation

Another application of the JavaScript programming in Acrobat is the creation of simple animations. Figure 4 has several GUI controls to manage the molecular scene. The check box shows/hides displacement vectors associated with selected vibration while two buttons, "Animate" and "Stop", toggle animated display of the motion

corresponding to the selected vibration. The molecule can be rotated and zoomed during the animation.

Creating dynamic content within Acrobat using JavaScript is not always straightforward and simple but it gives the author new abilities to expand the scope of PDF beyond the static content and to also convey some information crucial for in-depth understanding to the reader. In the meantime, we have developed several on-line tutorials [7] which can be used for creating dynamic Acrobat content for the general case scenarios by users inexperienced in JavaScript. Tutorials include step by step instructions and sample JavaScript code which can be copied and pasted into the Adobe Acrobat.

4 Conclusions

We have demonstrated with our examples that PDF is not just a medium for exchanging and viewing the static 2D electronic documents. The PDF capabilities can be greatly expanded by embedding the 3D interactive models which can be viewed and manipulated by the reader without the specialized visualization software. Furthermore, the Acrobat JavaScript coding allows creation of the dynamic 3D content where an end user can interact with Acrobat using GUI controls. Thus, PDF documents with integrated 3D models provide new ways of visualizing complex molecular properties in an instructive and interactive manner which is ideally suited for the research and educational purposes.

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