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Development of RYUGA for three-dimensional dynamic visualization of molecular dynamics results

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Abstract

We have developed a new computer graphics (CG) code RYUGA for three-dimensional dynamic visualization of molecular dynamics (MD) results. The applicability of RYUGA for visualizing and analyzing the dynamics of atomic motions in various materials was demonstrated. RYUGA supports various functions, such as solid-modeling CG pictures (called the CPK model), CG animation of the MD results, Miller plane cutting of crystal structures, building graphs, etc., similar to other CG codes for MD simulation. In addition, RYUGA has a number of advantages as follows: (i) a perspective is employed for drawing CG pictures, (ii) three-dimensional trajectories of atoms can be constructed, (iii) an operator can travel inside the materials, (iv) graphic speed and animation speed are enhanced because of the specific algorithms, and (v) it works on any workstations, moreover even personal computers with a UNIX operating system and an X window system are available.

1. Introduction

Computer-assisted material design is a new area of chemistry which has been brought about by significant advances in computer technology and theoretical chemistry, such as quantum chemistry (QC), molecular dynamics (MD), molecular mechanics (MM), artificial intelligence (AI), and data base (DB) management [1–3]. Although it is desirable that experimental researchers employ computer calculations as an ordinary tool for the design of novel materials, only very few specialists actually apply computational chemistry to material design. One of the complexities and difficulties of computational chemistry is the analysis of the huge numerical output that is obtained from the computer calculations. Recently, the application of computer graphic (CG) techniques to the analysis of the computer calculation results has revolutionized the general image of computational chemistry, because it simplifies and effectively displays the results of the computer calculations. In other words, computational chemistry has become popular due to the introduction of the CG technique.

Of the various computational techniques, MD is popular for the study of the structure, dynamics, and physical properties of various substances. MD simulation has gained popularity due to the development of new algorithms and improved computer hardware facilities. Now more reliable results can be derived from MD methods, leading not only to the verification of concepts but also to the prediction of interesting new properties which

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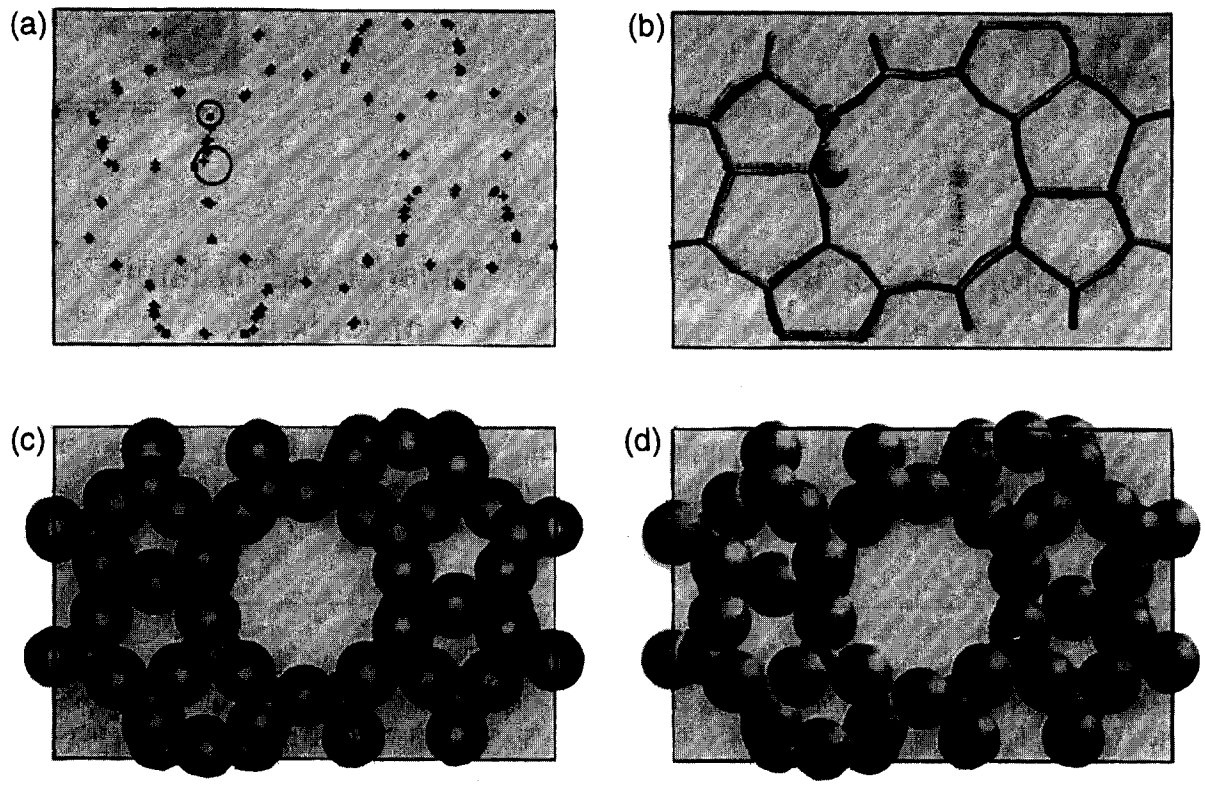

Fig. 1. CG pictures of Cu-ZSM-5 with several different display styles of atoms. (a) Dot model, (b) stick model, (c) CPK model, and (d) modified CPK model.

had never before been reported by analytical experiments. We confirmed the applicability of MD and CG methods to investigate the structures, dynamics, and functions of various materials including catalytic materials, zeolites, clays, ultrafine particles, oxide superconductor films, carbon nanotubes, supercritical fluids, etc. [4–8].

In the early days, the MOGLI code (Evans and Sutherland) was the most famous tool for producing static CG pictures of molecular and crystal structures. Since the CG animation of MD results could not be produced by MOGLI, the dynamics of atoms in materials could not be clarified. Moreover, since it worked only on an Evans and Sutherland three-dimensional color graphic terminal, it was a specific tool for researchers who were very interested in the CG technique. Recently, Insight (Biosym Technol. Inc.), CERIUS (Molecular Simulations Inc.), PolyGraf (Molecular Simulations Inc.), etc. were simultaneously developed for the CG visualization of molecular and crystal structures. Now the Insight and the CERIUS codes have been advanced to Insight II and CERIUS II, respectively, due to large improvements. Since these codes support a lot of functions, including CG animation of MD results, Miller plane cutting of crystal structures, building graphs, etc., they are very effective and efficient tools for the analysis of MD results. However, a significant problem has not been solved: only specific three-dimensional graphic workstations with a graphic board or graphic accelerator are available for these CG codes. This is a serious obstacle for the popularization not only of CG techniques but also of computational chemistry.

In 1991, we developed MOMOVIE on an OMRON LUNA88K workstation. Since it employed a specific algorithm for the enhancement of the animation speed, it worked on a standard workstation without a graphic board or graphic accelerator. Although MOMOVIE has had a great deal of impact on chemists, its func-

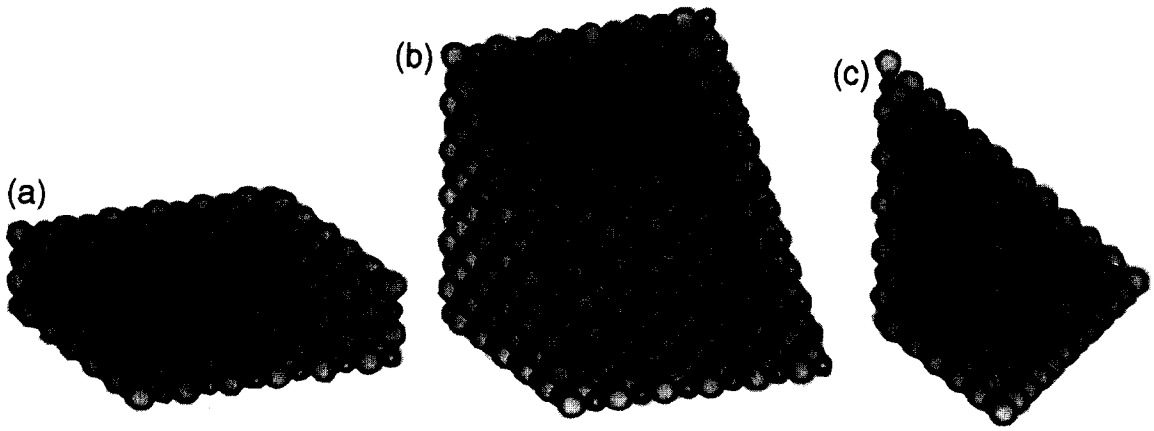

Fig. 2. CG picture of various MgO planes. (a) (100) plane, (b) (110) plane, and (c) (111) plane.

tions were very limited. In this study, we report on the development of a new multi-functional CG code RYUGA for three-dimensional dynamic visualization of MD results. We relate here a lot of advantages of RYUGA, and its applicability is demonstrated.

2. Environment

C language, Xlib, and X window systems were used for the development of RYUGA on a Hewlett-Packard HP9000 series model 715/33 workstation. We confirmed that X11 release 4 and 5

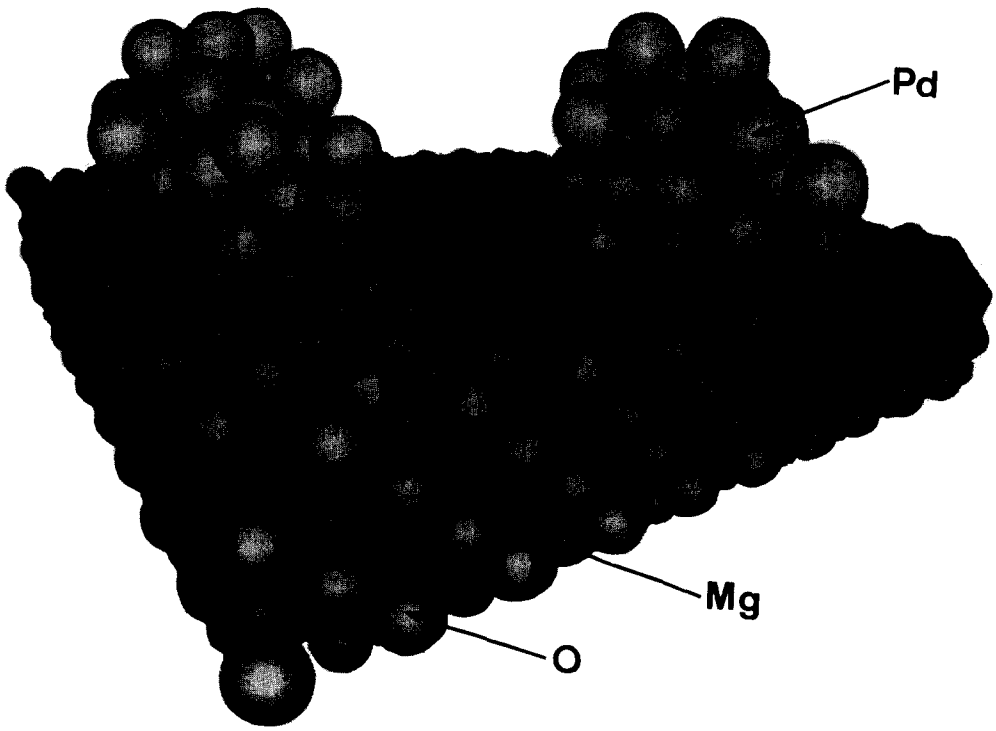

Fig. 3. CG picture of Pd clusters on MgO(100) plane drawn with a perspective.

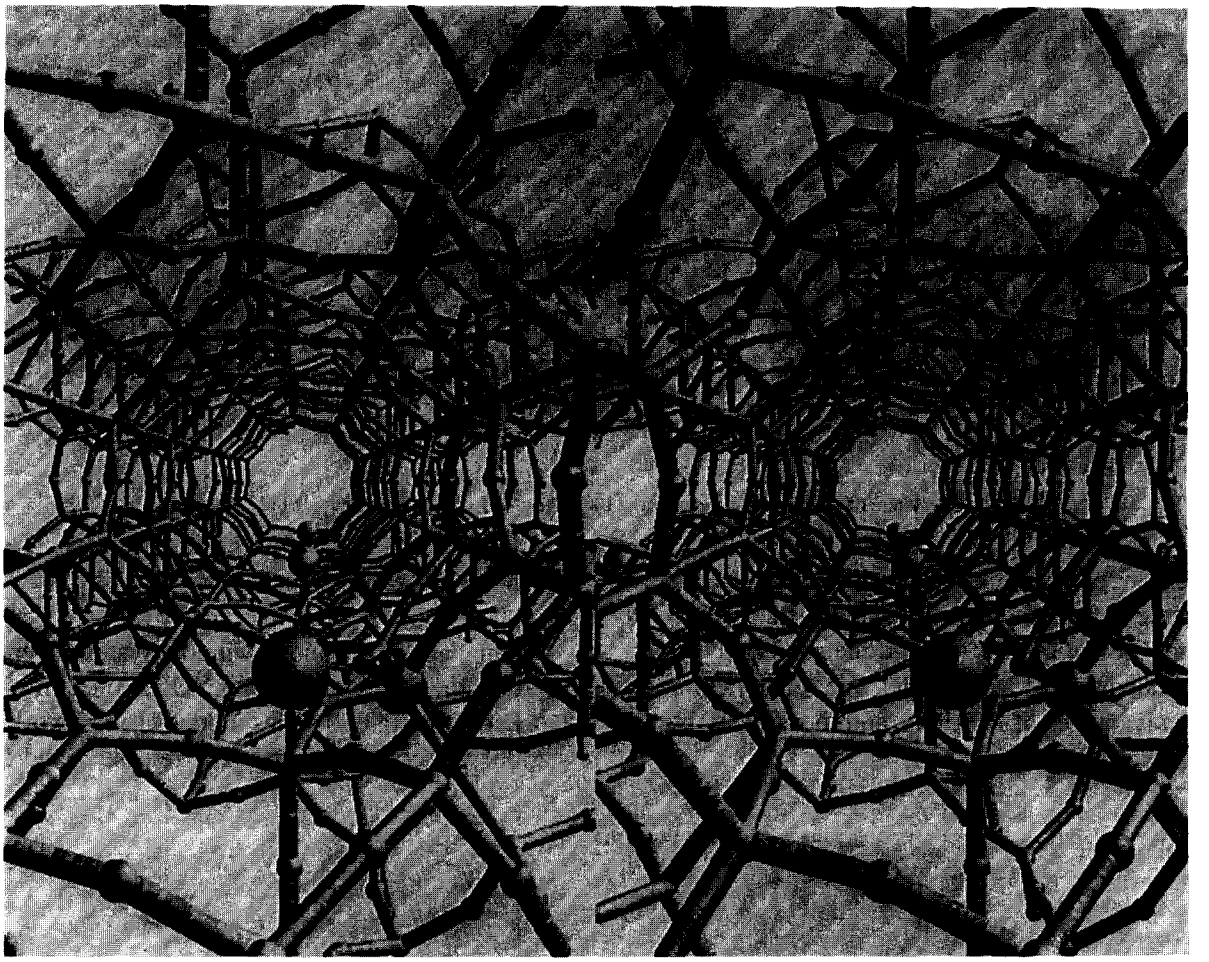

Fig. 4. Stereograph of Cu-ZSM-5 drawn with a perspective.

are available as an X window system for RYUGA. As architecture, a screen that displays more than 256 colors simultaneously and a mouse with three buttons are essential. Although at present RYUGA can visualize and analyze the MD results calculated with the MXDORTO or XDORTO codes developed by Kawamura [9], in the future MD results obtained by other MD codes will be available.

3. Multi-function

RYUGA has a number of effective and efficient functions for visualizing and analyzing the dynamics of atomic motions in various materials, similarly to other CG codes, such as Insight II and CERIUS II. Its general functions are described as follows:

(1) Solid modeling CG pictures of molecular and crystal structures can be made (called CPK model).

(2) CG animation of MD results can also be made with its three-dimensional CG technique.

(3) Several different display styles of atoms and bonds are available, such as the stick model, the ball model, and the CPK model (Fig. 1).

(4) The crystals can be cleaved at an arbitrary Miller plane to build slabs (Fig. 2).

(5) Various graphs of MD results, such as time vs. energy, time vs. temperature, and time vs. mean square displacements of atoms can be constructed.

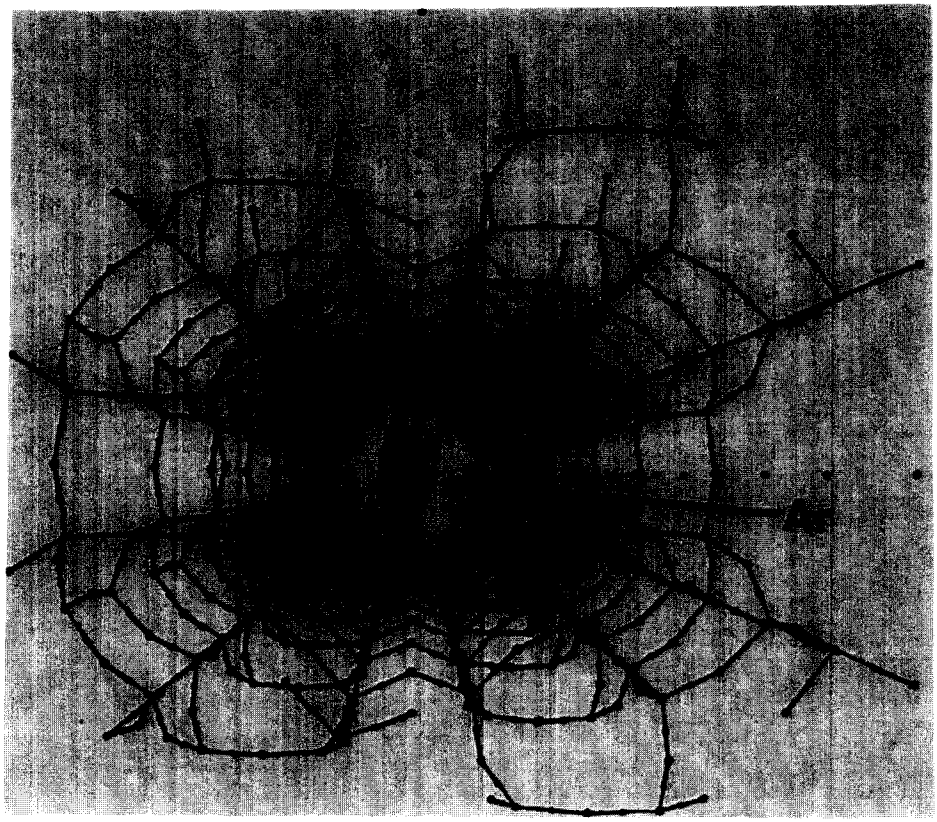

Fig. 5. Three-dimensional trajectory of Ar in Na-mordenite drawn with a perspective.

(6) Changes in the distance between two arbitrary atoms can be shown during the CG animation of the MD results.

(7) Titles and annotations can be displayed on the screen.

(8) Device drivers were developed to print the CG pictures on a Seiko D-scan CH4104 full-color printer and the trajectories of atoms on an HP-GL based plotter.

(9) Most functions can be operated by a mouse.

4. Advantages

In addition to the general functions described previously, RYUGA has a number of advantages compared to other CG codes for MD simulation. These are as follows.

4.1. Perspective

All CG codes for MD simulation, including RYUGA, employs a shading method for expressing the depth of the molecular and crystal structure as shown in Fig. 1. In addition, RYUGA employs a perspective to express the depth, as shown in Fig. 3. This method promotes a detailed understanding of the three-dimensional structure of complicated materials such as zeolites, proteins, and polymers. Moreover, the stereograph can also be constructed with a perspective (Fig. 4).

4.2. 3-Dimensional trajectory

Three-dimensional trajectories of atoms in materials that are obtained by MD simulation are effective for analyzing the dynamics of atomic motions, especially the behavior of various molecules in catalysts, adsorbents, or membranes.

Fig. 6. CG picture of faujasite as seen from the position of Na cation.

RYUGA can construct a three-dimensional trajectory with a perspective which cannot be produced by other CG codes (Fig. 5).

4.3. Travel inside the materials

Only a view from outside the materials can be constructed by other CG codes, whereas RYUGA can produce a view from an arbitrary point inside the materials to promote an atomistic understanding of the local structure (Fig. 6). An operator of RYUGA seems to travel inside the materials. The introduction of a virtual reality technique to computational chemistry is our dream so that atomic motions in various materials can be visualized and analyzed.

4.4. Specific algorithm for the enhancement of the graphic speed

Graphic speed is enhanced because of a specific algorithm. Other CG codes draw a huge amount of polygons for expressing one ball or one stick. Here, a ball and stick represent an atom and a bond, respectively, in the CG pictures of molecular and crystal structures. Although it is an effective method for producing CG pictures with a good quality and contrast, it takes too much CPU time. Therefore, a specific graphic workstation with a graphic board or graphic accelerator is indispensable for performing these CG codes. Since only balls and sticks are drawn in the CG picture of molecular and crystal structures, such sophisticated CG techniques as polygon drawing

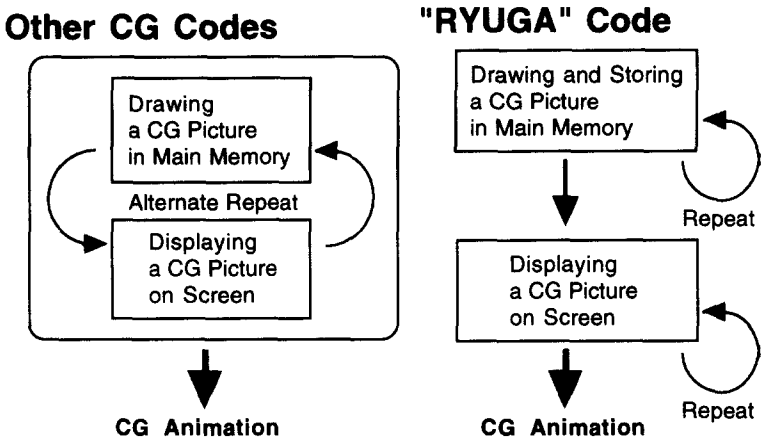

Fig. 7. Specific algorithm for the enhancement of the animation speed.

are not actually essential for these MD codes. The refined technique is required only for drawing complicated CG pictures, such as a human face, animal, and landscape. RYUGA employs a simple and specific algorithm for drawing CG pictures. In detail, 16 concentric rings are drawn for expressing one ball, instead of drawing a number of polygons. Since this specific algorithm enhances the graphic speed of RYUGA, a specific graphic workstation is not indispensable for the use of RYUGA.

4.5. Specific algorithm for the enhancement of the animation speed

Animation speed is also enhanced because of another specific algorithm. When a CG picture is drawn on the screen, two procedures are generally performed. The first procedure is drawing the CG picture in the main memory of the workstation, and the second one is transforming the completed CG picture from the main memory to the screen. During the drawing of the next CG picture in the main memory, the previous CG picture still remains on the screen. Here, the first one is called the drawing procedure and the second one is called the display procedure. In other CG codes, the drawing procedure and the display procedure are alternately repeated for producing the CG animation of MD results. However, the CG animation does not seem to be continuous and it lacks the reality on a standard workstation which has a low graphic speed. To solve this problem, RYUGA employs a new specific algorithm. In RYUGA, two procedures are performed for the production of the CG animation. The first procedure is drawing and storing a number of CG pictures in the main memory of the workstation, and the second one is the continuous transformation of stored CG pictures from the main memory to the screen one after another (Fig. 7). In RYUGA code, the display procedure is performed after the draw procedure is completed, namely the draw procedure is definitely separated from the display procedure. Since the draw procedure which is rate-determining step for producing CG animation is separated as a pre-procedure of CG animation, the speed of CG animation in RYUGA code is extremely fast even on a standard workstation without a graphic board and a graphic accelerator.

4.6. Transplantation

Other CG codes for MD simulation work on specific graphic workstations, such as Silicon Graphics and Titan workstations, because a high performance in drawing the CG pictures is essential for executing these CG codes. RYUGA code does not require a specific three-dimensional graphic workstation because of the enhancement of the graphic and animation speed, described previously. It works on standard workstations, more-

over even on personal computers with a UNIX operating system and an X window system are available. We confirmed that RYUGA can work on various workstations with a UNIX operating system and an X window system including the Hewlett-Packard workstation, the Sun workstation, and the Silicon Graphics workstation. Moreover, it also works on an IBM personal computer with a UNIX operating system, such as Linux. Other CG codes for computational chemistry were the exclusive tool of a small group of researchers. RYUGA may change the general image of the CG technique for computational chemistry and it may even promote the popularity of computational chemistry. Thus, in the future, CG techniques can be employed as an common tool for material design not only by computational chemists, but also by experimental chemists.

5. Future enhancements

A number of additions and enhancements are under consideration for future versions of RYUGA, including, for example, the visualization and analysis of quantum chemical calculations. Moreover, the introduction of the virtual reality technique to computational chemistry is our future dream, as described previously.

6. Availability

RYUGA has been registered at the Japan Chemistry Program Exchange organization (JCPE). A source file is distributed through JCPE, 2-4-16, Yayoi, Bunkyoku, Tokyo, Japan (fax: (+81-3)8167826, tel: (+81-3)8163581).

References

[1] M. Doyama, J. Kihara, M. Tanaka and R. Yamamoto (Editors), Computer-Aided Innovation of New Materials II, Elsevier, Amsterdam, 1993, pp. 985–1114, and references therein.
[2] H. Niiyama, T. Hattori and A. Miyamoto (Editors), Computer-Assisted Research for Catalyst Design, Elsevier, Amsterdam, 1991, and references therein.
[3] C.R.A. Catlow, P.A. Cox, R.A. Jackson, S.C. Parker, G.D. Proce, S.M. Tomlinson and R. Vetrivel, Mol. Simul., 3 (1989) 49, and references therein.
[4] A. Miyamoto, K. Takeichi, T. Hattori, M. Kubo and T. Inui, Jpn. J. Appl. Phys., 31 (1992) 4463.
[5] A. Miyamoto and M. Kubo, Stud. Surf. Sci. Catal., 83 (1994) 117.
[6] A. Miyamoto, R. Yamauchi and M. Kubo, Appl. Surf. Sci., 75 (1994) 51.
[7] A. Miyamoto, H. Himei, Y. Oka, E. Maruya, M. Katagiri, R. Vetrivel and M. Kubo, Catal. Today, 22 (1994) 87.
[8] M. Kubo, R. Yamauchi, R. Vetrivel, and A. Miyamoto, Appl. Surf. Sci., 82/83 (1994) 559.
[9] K. Kawamura, in F. Yonezawa (Editor), Molecular Dynamics Simulations, Springer Verlag, Berlin, 1992, p. 88.