Crystal Viewer: An Online Platform for Learning and Understanding Crystalline Structure

Yuanchen Chu[1,*], Daniel F Mejia[1], James Fonseca[1], Michael Povolotskyi[1] and Gerhard Klimeck[1]

[1]Network for Computational Nanotechnology, Purdue University, West Lafayette, IN 47907
*e-mail: chu72@purdue.edu

INTRODUCTION

Most materials found in nature have their atoms arranged in a regular and repeated pattern known as the crystalline structure. Crystals have a huge number of applications in science with one of them being the basis for all nanotechnology and microelectronics. It is very important to understand the crystalline structure of materials in order to study and predict their properties such as conductivity for electricity, conductivity for heat, optical properties and more. As a growing number of crystals with complex structures are being used in modern technology, students and scholars need a better way to visualize these crystals than plain text book pictures. The Crystal Viewer [1] deployed on nanoHUB [2] provides such a simulation platform for the research community through the web browser. The tool has the ability to visualize materials of different crystalline structures including diamond, zincblende, wurtzite, etc. It can also visualize the 14 Bravais lattices. Besides, it can create user defined crystalline structure with the basis and the lattice input by the user.

TOOL DESCRIPTION

Crystal Viewer tool is an excellent supplement to text book pictures of crystal materials. The crystalline structure that can be visualized by the tool ranges from diamond, zincblend, wurtzite to sodium chloride, cesium chloride, fcc, bcc and carbon meshes. Users can choose to use the conventional basis or the primitive basis and set the dimension of the crystal. Up to three miller planes can be drawn along with the crystal material. The tool can analyze the crystalline structure and choose an optimal shape of the plane and position to 'place' the plane. Alternatively, the user can manually set the position by entering the cross point on the axis. Although the tool can visualize a large number of materials, it is difficult to include all existing crystal materials. In order to overcome this limitation, a function has been developed for creating and viewing user defined crystals. The user can input any basis and lattice and the tool can then visualize the input structure. The miller plane can also be drawn along with the user defined crystals.

The tool runs within the Rappture interface [3] and uses NEMO5 [4] simulation tool in the background to perform calculations. Usage statistics [5] shows that more than 7000 users have run over 65,000 simulations.

CONCLUSION

An online platform for simulating crystalline structures has been shown. The tool has been deployed on nanoHUB and can visualize different crystal materials along with the miller plane, the 14 Bravais lattices and create user defined crystalline structures. It is acting as a research and learning tool for the scientific and educational community.
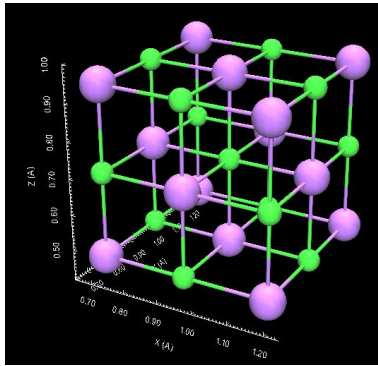
ACKNOWLEDGEMENT

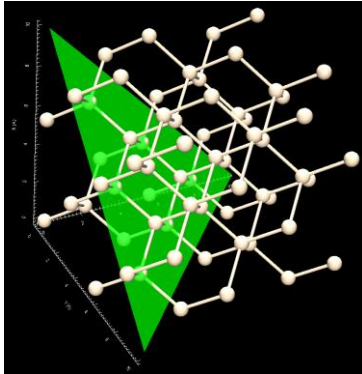Fig. **1**. Visualization of a NaCl unit cell

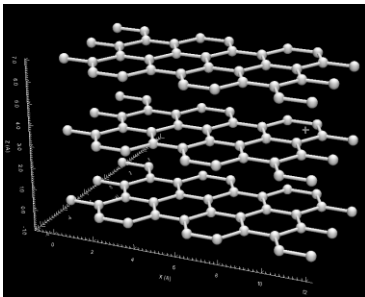Fig. 2. Visualization of diamond structure material silicon with a (111) plane
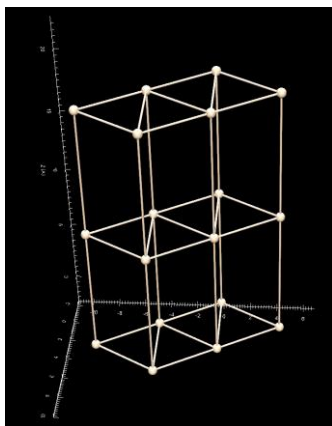

Fig. 3. Visualization of 3 graphene layers

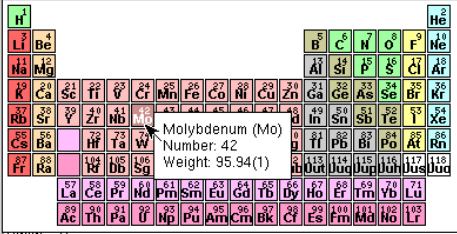Fig. 4. The hexagonal Bravais Lattice

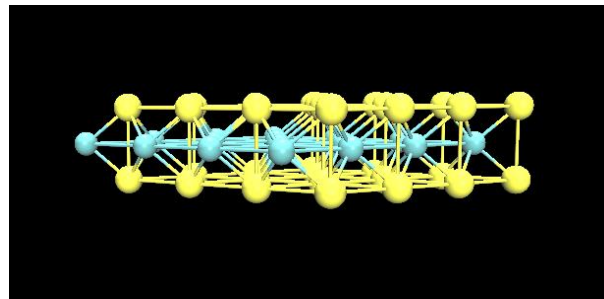Fig. 4. The menu for setting user defined crystals

Fig. 5. Visualization of dichalcogenide structure material Molybdenum disulfide (MoS_2) using the function of user defined crystal

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    doi:10.4231/D3VT1GQ8M
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[5] https://nanohub.org/resources/crystal_viewer/usage