

Developing a Crystal Viewer Tool for nanoHUB

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Most materials found in nature have their atoms arranged in a regular and repeated pattern known as crystalline structure; this is particularly true for metals. It is very important to understand the crystal structure of materials in order to predict their properties such as the electric conductivity, heat transfer, and more. Particularly, students and scholars in the field of material science need a way to visualize the different crystal structures. Atomic structures of elements are not visible to the naked eye. In that context, a computer based tool can be used to simulate and to visualize the crystal structures of different elements. Nanohub is a web-based workspace that offers multiple simulation tools for nanotechnology scientists all around the world. This project intends to develop a tool to view crystal structures, similar to the tools already available on nanohub, where users can select the material they want and output its 3D structure. Fortunately, Nanohub has a built-in workspace “rappture” to develop user-interfaces for new tools. As for now, an intuitive user-interface has been developed and the code used to run the simulations is currently under progress. Ultimately, a decent Crystal Viewer will be available to use on Nanohub allowing users, ranging from high school students to undergraduate students and faculty members, to view a wide range of structures for most of the useful materials using Crystal Viewer. However, this tool has limited features for advanced usage which leaves room for future improvement.