

Next Generation Crystal Viewing Tool

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The science and engineering community is limited when it comes to crystal viewing software tools. Each tool lacks in a different area such as customization of structures or visual output. Crystal Viewer 2.0 was created to have all of these features in one program. This one tool simulates virtually any crystal structure with any possible material. The vtkvis widget offers users advanced visual options not seen in any other crystal viewing software. In addition, the powerful engine behind Crystal Viewer 2.0, nanoelectronic modeling 5 or (NEMO5), performs intensive atomic calculations depending on user input. A graphical user interface, or GUI, is created using rappture (rapid application infrastructure) that creates a driver file that is subsequently sent to a wrapper to create an input deck to NEMO5. NEMO5 helps to generate a vtk file that is sent back to the wrapper to generate a run file. Rappture in turn runs the file and generates another vtk file for the vtkvis widget. This widget sends the data to a rendering server that generates the final rendering to be output on the user interface. The final result is a rotatable crystal lattice structure that can be saved and viewed later if necessary. Crystal Viewer 2.0 is a prime candidate for students in introductory materials science courses and can be accessed via nanohub.org all over the world in the near future.