

Visualization of Oxidation Reduction Simulations

Visualization is an effective method of explaining the unexplainable, depicting the invisible, and exploring complicated relationships. In nano-science, visualization has been used to explore and explain the many uses of carbon nanotubes since its discovery in 1991 by Sumio Iijima. A framework was developed and applied for visualizing, simultaneously, on a tiled-display or on a powerwall, the results of two simulations locked in step. The framework is applied to visualize and then compare the results of two simulation's approaches to determine the minimal energy required for oxidation reduction involving methane and a carbon nanotube.

The output is post-processed and visualized from molecular dynamics simulations and from quantum mechanical simulations. A combination of computer graphics software packages, VMD, XDMX, and Blockbuster, are used to visualize the effects of heating on a nanotube simulated using the two methods. A PC cluster was setup using three dual processor computers. These three computers' graphics cards are used to drive six LCD panels. The XDMX package was used to run a single X-server across the LCDs to create a unary display. The software package VMD is used to generate the 3D visual images of the molecular simulations as well as the quantum simulations. VMD is also used to create the movie files that Blockbuster would run on the tile display. The LCD displays show the molecular simulation in the center of the screen surrounded by fragments of the simulation based upon temperature, as well as views of the quantum simulation data.

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