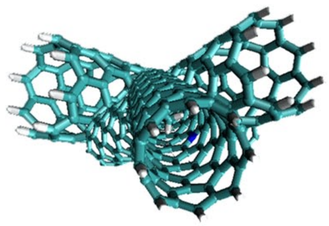
# *Visualization of Oxidation-Reduction for Methanol Production*

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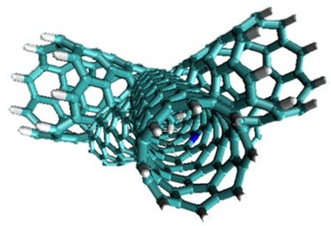
***http://www.csm.ornl.gov/Internships/Websites05/j_montgomery/abstract.html***



## Research Goals

- Use parallel computing and visualization techniques to analyze, render and display large scale datasets
- Analyze hundreds of gigabytes of data and rendering them results in a timely fashion
- Develop and integrate a framework and software to view simultaneously two different simulations of an oxidation-reduction process for methanol production
- Parallel computing using the central processors and the graphics processors are performed.
- The framework and software is general and can be used in most tiled displays and powerwalls driven by clusters of workstations.

## Results

- Analysis and isosurface representation of data contributed to the process of scientific discovery.
- Visualization assisted in the discovery of excess charge density around the nitrogen in the nanotube.
- Simulation and analysis are continuing to study oxidation-reduction involving carbon nanotubes.

Using the test cluster and the tiled LCD display, simultaneous views of a quantum nanotube simulation (bottom left and right structures) and a molecular dynamic simulation (top left and right images) are displayed. Nanotube configurations at different temperatures are displayed in the center column.

1. VMD is a licensed software of the University of Illinois, and was developed by the theoretical and Computational Biophysics Group and the NIH Resource for Macromolecular Modeling and Bioinformatics.

http://www.ks.uiuc.edu/Research/vmd/

2. Xdmx is a open source project being collaborated on by many different programmers. This software eliminates the limitations of graphics devices being located on the same physical machine.

http://dmx.sourceforge.net/

The module and framework has been demonstrated on the ORNL EVEREST powerwall. The orange isosurfacing denotes the charge density from the quantum simulations. Scientist were able to find an excess of charge density where oxidation reductions is taking place (around the nitrogen defect and the oxygen in the methane molecule).

## Methodology

- **Constructing a testing cluster**
  - Software was developed, installed and configured for a prototype cluster of 3 PCs, each with a high-end graphics card which powered 6 LCD panels for a 2x3 11 megapixel display.
- **Create a unary display across the LCDs**
  - XDMX was implemented as a means of allowing the GPUs in the cluster to communicate with each other and work together in producing the display.
- **Visualization of the simulations**
  - VMD was used to render each simulation's data separately based upon the important specifics of that simulation. By doing this a script was generated to render the simulation repeatedly.
- **Bridge the XDMX and VMD modules**
  - An interface module was written to bridge XDMX and VMD to allow simultaneous viewing of VMD displays of nano-structure simulations.

## Summary

- Software framework was developed to display, simultaneously, two different simulations
- Tool that permits a high level of interactivity in visualizing both quantum mechanical based and molecular dynamics based simulations
- Infrastructure is portable and has been demonstrated on the ORNL powerwall.

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