Molecular Dynamics Simulations of Methanol in Single-Walled Carbon Nanotubes (SWNTs)

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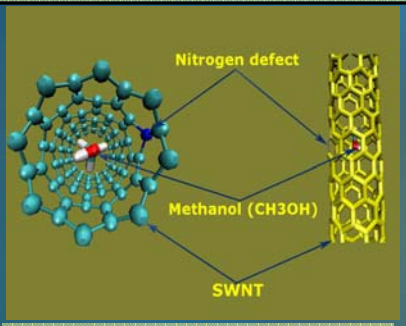
http://www.csm.ornl.gov/Internships/rams_05/abstracts/j_solomon.pdf

Abstract

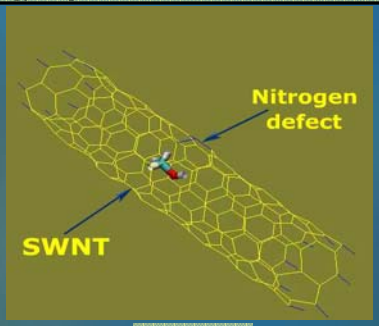
Molecular Dynamics Simulation is an extremely powerful method which involves solving problems in contexts relevant to the study of matter at the atomic level. It is a technique where the time evolution of the molecular system is followed by integrating their equations of motion providing the actual trajectory of the system. The output from the quantum and classical molecular dynamics simulations were used to investigate the dynamics and behavior of Methanol (CH_3OH) inside a zigzag (8,0) Single-Walled Carbon Nanotubes (SWNTs). At the start of all the simulations, methanol is placed near a "defect nitrogen" in an open nanotube and the system is simulated at various temperatures. In broadest sense, it is difficult to detect and determine the properties of molecules inside nanotubes therefore computational methods such as molecular dynamics simulations were applied to determine the thermal properties of atoms inside the carbon nanotubes. At low temperatures, the methanol molecule remains inside the nanotubes having low diffusion rate. However as the temperature rises, it starts to vibrate and rotate with varying arrays of motion. These results predict the specific temperature and rate the molecule diffuses out of the carbon nanotube. The simulations also indicate the manner and dynamics of the CH_3OH molecule in nanotubes while quantum calculations determine the minimal energy required for oxidation reduction of chemical changes in SWNTs.

Project Goals/Tasks

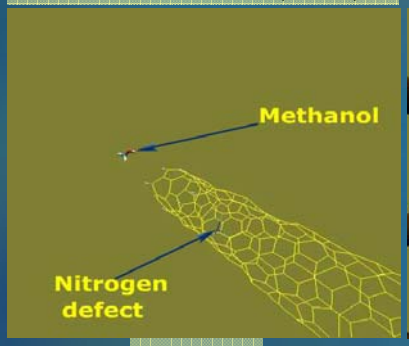
- Determine the catalytic effect of a "nitrogen defect" has on a methanol molecule
- Stimulate the encapsulated molecule inside a Single-Walled Carbon Nanotube (SWNT) using molecular visualization programs
- Use heat as a primary stimulus
- Observe how a single defect in the SWNT affects the interaction of the nanotube in different strenuous situations
- Determine specific temperature where the interactions (i.e. hydrogen bonds) inside the SWNT break
- Study the thermal property of methanol, to reduce the energy needed to break up methanol to H_2 and CO inside the SWNTs



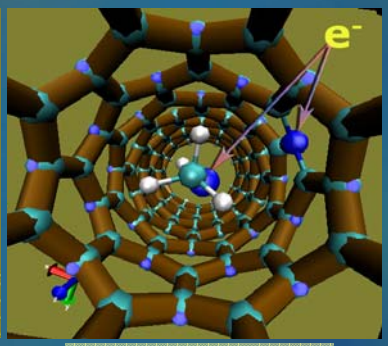
Implementation of Methanol in Single Walled Carbon Nanotube (SWNT)



800 Kelvin



2500 Kelvin



Isosurface of 300 Kelvin

Single-Walled Carbon Nanotubes (SWNT)

- Tiny stripes of graphite sheets rolled into a seamless cylinder
- Types:
  - armchair (n,n)
  - chiral (2n,n)
  - zigzag (n,0)
- Can stand repeated buckling and twisting
- Has high thermal conductivity, suitable for heat removal applications
- Can conduct electricity like copper
- Act as a semiconductor as silicon
- Transport heat as good as diamond in room temperature

Simulation Method

- Classical molecular simulations were used to investigate the dynamics and behavior of methanol (CH_3OH) in SWNTs with a nitrogen defect
- Temperature is used as a variable
- Pressure is kept constant throughout
- Software packages used for Simulation:
  - Tinker
  - VMD (Visual Molecular Dynamics)

Results/Conclusion

- The methanol (CH_3OH) molecule diffuses out of the SWNT in a spiral manner as the temperature increases; hence, around 2200 K.
- As the temperature rises, the charges on the nitrogen reacts with the oxygen forming a bundle. Hence, the energy inside the nanotube tries to break the interactions surrounding the molecule (e.g., hydrogen bonds) apart and eventually pushing the methanol molecule out of the SWNT.
- The energy calculated will help in the minimize energy needed to break up methanol to H_2 and CO inside SWNTs.
- $CH_3OH \rightarrow\!\!\leftarrow 2H_2 + CO$, $\triangle H^0_{298}$ is 92.0 kJ/mol^{-1}. However, inside SWNTs, it will be nearly 20 kJ/mol^{-1} after the specific temperature where it diffuses calculated..

Future Potential Applications

- Used for fuel cells to replace batteries in portable electronics
- SWNTs serve as field effect and single electron transistors
- Methanol is the most promising alternative automobile fuels from a non petroleum source
- **DOE** applications:
  - Use methanol as the best storage medium for H_2 fuels
  - Conducting composites
  - Thin film lithium ion batteries
  - Polymeric thin film solar cells

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