



# Carbon Nanotubes in Water

Simulate the behavior of carbon nanotubes immersed in aqueous environments.

Carbon nanotubes (CNT) are novel structures with unique mechanical and electrical properties, with prospective applications in fuel storage, sensor technology, and surface science. At CSE Lab, we are continuously developing a parallel molecular dynamics code (FASTTUBE) that allows large scale computations of CNTs interacting with water.

Two projects are offered:

The first project involves the simulation of a carbon nanotube operating as a tip of an Atomic Force Microscope, penetrating and oscillating through a free surface of water. The work includes a short literature survey on the AFM technique, performing the simulation as well as analyzing and visualizing the results.

The second project concerns nonequilibrium molecular dynamics simulations of the thermal conductivity of carbon nanotubes immersed in water. In this project we will interact with experimental groups conducting relevant studies

This project is in close collaboration with Dr. R. L. Jaffe at NASA Ames, USA.

## PREREQUISITES

Programming experience (F90)  
Experience in using Linux/UNIX  
Interest in Nanotechnology  
Independent work

## CONTACT

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