

## **Singapore Stanford Partnership Programme**

### **MS Project MS08-11**

#### **High Flux Membranes for Water Purification Systems: Molecular Simulations**

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The objective of this project is to develop computational models of high flux carbon nanotube membrane systems. The computational modeling endeavors to contribute fundamental knowledge regarding the nature of transport phenomena in high flux nanotube membranes. The system of interest in this research project is a carbon nanotube membrane that comprises an array of carbon nanotubes aligned vertically within a substrate of impermeable material. The carbon nanotube pore sizes will be on the order of less than 10 nanometers. The modeling study will investigate applications for desalination where water containing salt ions ( $\text{Na}^+$  and  $\text{Cl}^-$ ) is filtered through the membrane. The objective of the system is to achieve high flux of water molecules while excluding permeation of the salt ions.

Pre-requisite: the student must have very strong background in computer programming and molecular computational techniques.