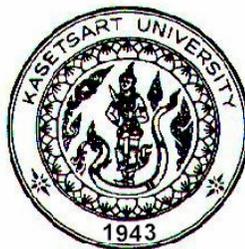


**THESIS**

**STRUCTURE AND DYNAMICS OF WATER CONFINED  
IN SINGLE-WALLED NANOTUBES: A MOLECULAR  
DYNAMICS STUDY**

**NONGNUCH ARTRITH**

**A Thesis Submitted in Partial Fulfillment of  
the Requirements for the Degree of  
Master of Science (Chemistry)  
Graduate School, Kasetsart University  
2008**



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**TITLE:** Structure and Dynamics of Water Confined in Single-Walled Nanotubes:  
A Molecular Dynamics Study

**NAME:** Miss Nongnuch Artrith

**THIS THESIS HAS BEEN ACCEPTED BY**

THESIS ADVISOR

( Assistant Professor Piboon Pantu, Ph.D. )

COMMITTEE MEMBER

( Professor Jumras Limtrakul, Ph.D. )

COMMITTEE MEMBER

( Mr. Tanin Nanok, Ph.D. )

DEPARTMENT HEAD

( Associate Professor Noojaree Prasitpan, Ph.D. )

**APPROVED BY THE GRADUATE SCHOOL ON** \_\_\_\_\_

DEAN

( Associate Professor Vinai Artkongharn, M.A. )

Nongnuch Artrith 2008: Structure and Dynamics of Water Confined in Single-Walled Nanotubes: A Molecular Dynamics Study. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Assistant Professor Piboon Pantu, Ph.D. 78 pages.

Structures and dynamics of water molecules in nanoporous media exhibit interesting characteristics different from their ordinary bulk properties and may lead to potential applications in sophisticated nanofluidic devices. In this study, molecular dynamics simulations were performed to investigate water molecules confined in single-walled carbon nanotubes (SWCNTs) and boron nitride nanotubes (SWBNNTs). Water density of  $1.00 \text{ g cm}^{-3}$  was placed inside the models of (*n,n*)-armchair nanotubes with different diameters ( $n = 9, 10, 12, 14, 16$  and  $20$ ) and the simulations were performed in the canonical *NVT* ensemble at  $298 \text{ K}$  by using the Nosé-Hoover thermostat in DL\_POLY program package. The wall-water interactions were varied within reasonable limits by changing the strength of the Lennard-Jones (LJ) parameters. Distribution functions were reported for the water in the tubes in spherical and cylindrical coordinates and the single-molecule dynamics, in particular self-diffusion, were monitored. While this motion was very much slowed down in narrow tubes, in keeping with previous findings (Mashl, R.J. *et al.* 2003 Nano Lett. 3(5):589-592.), bulk-water like self-diffusion coefficients were found in wider tubes. Axial diffusion coefficient increased with increasing tube diameter and reached its bulk value in the widest tubes with diameters of about  $24 \text{ \AA}$ . The convergence was faster for smaller wall-water interactions. An anomaly is, however, found for the SWBNNTs where the convergence was not monotonous.

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Student's signature

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Thesis Advisor's signature

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## LIST OF ABBREVIATIONS

Dz	=	Self-diffusion coefficient (z axis)
BLYP	=	Beck-Lee-Yang-Parr functional
BN	=	Boron nitride
BNNTs	=	Boron nitride nanotubes
CNTs	=	Carbon nanotubes
GlpF	=	Glycerol the crystal structure (F is symbol of native glycerol)
HF	=	Hartree-Fock
I <sub>x</sub>	=	Angular momentum x component
I <sub>y</sub>	=	Angular momentum y component
I <sub>z</sub>	=	Angular momentum z component
LJ	=	Lennard-Jones
MC	=	Monte Carlo
MD	=	Molecular dynamics
MSD	=	Mean square displacement
MWCNT	=	Multi walled carbon nanotube
n(r)	=	Coordination number
NPT	=	Isothermal-Isobaric (NPT) ensemble
NT	=	Nanotubes
NVE	=	Microcanonical ensemble (NVE)
NVT	=	Canonical ensemble (NVT)
PW	=	Plane-Wave
RDF	=	Radial distribution function
SPC	=	Simple point charge
SPC/E	=	Extended simple point charge
STM	=	Temperature scanning tunneling microscope
SWBNNT	=	Single walled boron nitride nanotube
SWCNT	=	Single walled carbon nanotube
TEM	=	Transmission electron microscopy