LIST OF ABBREVIATIONS

AM1	=	Austin Model 1
B3LYP	=	Becke's three parameters hybrid functional using the Lee-Yang-Parr correlation functional
BSSE	=	Basis set superposition error
CNT	=	Carbon nanotube
Cl^-	=	Chloride anion
DFT	=	Density functional theory
dSWNT	=	Defect single-walled carbon nanotube
ΔEa	=	Activation energy
FAU	=	Faujasite
FER	=	Ferrierite
FTIR	=	Fourier transform infrared spectroscopy
HF	=	Hartree-Fock
INDO	=	Intermediate neglect of differential overlap
KS	=	Kohn-Sham
LM	=	Local minimum
MFI	=	Mobil five zeolite
MM	=	Molecular mechanics
MNDO	=	Modified neglect of diatomic overlap
MO	=	Molecular orbital
MOR	=	Mordenite
MP2	=	The second-order Møller-Plesset perturbation theory
MWNT	=	Multi-walled carbon nanotube
NICS	=	Nuclear independent chemical shift
NNDO	=	Neglect of diatomic differential overlap
ONIOM	=	Our own n-layered integrated molecular orbital and molecular mechanics
PES	=	Potential energy surface
PM3	=	Parameterized Model 3

LIST OF ABBREVIATIONS (Continued)

pSWNT	=	Perfect single-walled carbon nanotube
QM	=	Quantum mechanics
QM/MM	=	Quantum mechanical/molecular mechanical
SW	=	Stone-Wales
SWNT	=	Single-walled carbon nanotube
TS	=	Transition structure
UFF	=	Universal force fields
ZSM-5	=	Zeolite socony mobil 5