LIST OF ABBREVIATION

B3LYP	=	Becke's three parameter hybrid functional using the Lee-Yang-Parr correlation functional
BSSE	=	Basis set superposition error
CP	=	Counterpoise method
DFT	=	Density functional theory
DOS	=	Density of states
FAU	=	Faujasite
FTIR	=	Fourier transform infrared spectroscopy
GGA	=	Generalized gradient approximation
HF	=	Hartree Fock
HOMO	=	Highest occupied molecular orbital
IMOMO	=	Integrated molecular orbital-molecular orbital
KS	=	Kohn-Sham
LCAO	=	Linear combination of atomic orbitals
LDA	=	Local density approximation
LPDOS	=	Layer-projected density of states
LUMO	=	Lowest unoccupied molecular orbital
MFI	=	Mobile Five zeolite
MM	=	Molecular mechanics
MP2	=	The second-order Møller-Plesset perturbation theory
ONIOM	=	Our Own N-layered Integrated molecular Orbital and molecular Mechanics
PDOS	=	Partial density of states
POAV	=	π-orbital axis vector analysis
QM	=	Quantum mechanics
QM/MM	=	Quantum mechanical/molecular mechanical
QM-Pot	=	Combined Quantum Mechanics - Interatomic Potential Functions

LIST OF ABBREVIATION (cont'd)

SCREEP	=	Surface Charge Representation of the Electrostatic Embedding Potential
T	=	Tetrahedral center
TDOS	=	Total density of states
TPD	=	Temperature programmed desorption
UV-Vis	=	UV-visible spectroscopy
XANES	=	X-ray absorption near-edge structure
XRD	=	X-ray diffraction
ZPE	=	Zero-point energy
ZSM-5	=	Zeolite Socony Mobil 5