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LIST OF ABBREVIATIONS

B3LYP	=	Becke's three parameter hybrid functional using the LYP correlation functional
BLYP	=	Beck-Lee-Yang-Parr functional
EXAFS	=	Extended X-ray Adsorption Fine Structure
DFT	=	Density Functional Theory
K	=	kelvin
kcal/mol	=	kilocalorie per mol
LANL2DZ	=	Los Alamos National Laboratory 2-Double-Zeta
LDA	=	Local Density Approximation
LSD	=	Local Spin Density approximation
MAS NMR	=	Magic Angle Spinning Nuclear Magnetic Resonance
MFI	=	Mobile Five framework type code
MM	=	Molecular Mechanics
MO	=	Molecular Orbital
ONIOM	=	Our own N-layered Integrated molecular Orbital and molecular Mechanics
ONIOM2	=	Our own two-layered Integrated molecular Orbital and molecular Mechanics
PND	=	Powder Neutron Diffraction
QM	=	Quantum Mechanics
QM/MM	=	Quantum Mechanics/Molecular Mechanics
SCF	=	Self-Consistent Field
SCREEP	=	Surface Charge Representation of External Embedded Potential Method

LIST OF ABBREVIATIONS (Cont'd)

STO-3G	=	Slater Type Orbital approximated by 3 Gaussian type orbitals
TMP	=	Trimethyl Phosphene
TS-1	=	Titanium Silicalite-1
UFF	=	Universal Force Field
VDW	=	van der Waals
XRD	=	X-ray Diffraction
ZSM-5	=	Zeolite Socony Mobil 5