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### LIST OF ABBREVIATIONS

SWNTs	=	Single-wall carbon nanotubes
MWNTs	=	Multi-wall carbon nanotubes
B3LYP	=	Beck's three parameter hybrid functional
		using the LYP correlation functional
AM1	=	Austin Model 1
ONIOM	=	The Our own N-layered Integrated
		molecular Orbital molecular Mechanics
kcal/mol	=	kilocalorie per mol
eV	=	electron volt
НОМО	=	Highest Occupied Molecular Orbital
LUMO	=	Lowest Occupied Molecular Orbital
Eg	=	Energy gap
Ea	=	Activation energy
Er	=	Reaction energy
В	=	Boron
Ν	=	Nitrogen
NPA	=	Natural Population Analysis
TS	=	Transition state
OPT	=	Optimization
QST3	=	Synchronous transit-guided quasi-Newton
		methods