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LIST OF ABBREVIATIONS

B	=	Boron
B3LYP	=	Beck's three-parameter hybrid functional using the LYP correlation functional
CNTs	=	Carbon nanotubes
CVD	=	Chemical vapor deposition
DOSs	=	Density of states
E _g	=	Energy gap
eV	=	electron volt
HOMO	=	Highest Occupied Molecular Orbital
I _h	=	Icosahedral
IPR	=	Isolated-pentagon rule
kcal/mol	=	kilocalorie per mole
LUMO	=	Lowest Occupied Molecular Orbital
MWCNTs	=	Multi-walled carbon nanotubes
N	=	Nitrogen
NPA	=	Natural Population Analysis
OPT	=	Optimization
PAPR	=	Pentagon adjacency penalty rule
PEG	=	Poly(ethylene glycol)
SWCNTs	=	Single-walled carbon nanotubes