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LIST OF ABBREVIATIONS

2D	= Two-dimensional
AIMD	= Ab initio molecular dynamics
Al ₂ S _n	= Aluminum polysulfide species
CI-NEB	= Climbing image-nudged elastic band
CNF	= Carbon nanofiber
COHP	= Crystal orbital Hamilton population
Cu-BHT	= Copper-benzenehexathial
DA	= Dual atom
DFT	= Density functional theory
DOS	= Density of states
E _{ads}	= Net adsorption energy
E _b	= Binding energy
E _{def}	= Deformation energy
E _{int}	= Intrinsic interaction energy
EMIM	= 1-ethyl-3-methylimidazolium
GGA	= Generalized gradient approximation
HF	= Hydrofluoric acid
ICOHP	= Integrated Crystal Orbital Hamilton Population
LDA	= Local density approximation
LIB	= Li-ion battery
MIM	= 1-butyl-3-methylimidazolium
NEB	= Nudged elastic band
NPs	= Nanoparticles
PAW	= Projector-augmented wave
PBE	= Perdew-Burke-Ernzerhof
PDOS	= Projected density of states
QM	= Quantum mechanical

LIST OF ABBREVIATIONS (Continued)

S_8	= Polysulfide
SA	= Single atom
SAC	= Single-atom catalyst
SCF	= Self-consistent field
SOAP	= Smooth Overlap of Atomic Positions
SRR	= Sulfur reduction reaction
SWCNT	= Single-walled carbon nanotube
TM	= Transition metal
VASP	= Vienna Ab initio Simulation Package
vdW	= van der Waals
V_O	= Oxygen vacancy
XC	= Exchange-correlation
η^{SRR}	= Overpotential for sulfur reduction reaction s