

Abbreviations

Abbreviation	Meaning
CN	graphitic Carbon Nitride, tri-s-triazine- $g-C_3N_4$, heptazine- $g-C_3N_4$
$BL-CN$	Bilayer of $g-C_3N_4$
$Li-CN$	Lithium intercalated Bilayer $g-C_3N_4$
TM	Transition Metal
E_F	Fermi Energy
NHE	Normal Hydrogen Electrode
E_{vac}	Vacuum Energy
Φ	Work function
η^{HER}	Overpotential for HER
η^{OER}	Overpotential for OER
HER	Hydrogen evolution reaction
OER	Oxygen evolution reaction
CO_2RR	Carbon dioxide reduction reaction
N_2RR	Nitrogen reduction reaction
E_{VB}	Valence band edge
E_{CB}	Conduction band edge
$TM-CN$	Transition Metal decorated $g-C_3N_4$
Hf_2CO_2/CN	Hf-based MXene supported $g-C_3N_4$
GGA	Generalized gradient approximation
SCF	Self consistent field
PBE	Perdew Burke-Ernzerhof
HSE	Heyd-Scuseria-Ernzerhof

vdW	van der Waals
DFT	Density functional theory
E_{BGC}	Band gap centre energy
VBM	Valence band maxima
CBM	Conduction band minima
ΔG^{HER}	Reaction barrier for HER
ΔG^{OER}	Reaction barrier for OER
$e^- - h^+$	Electron Hole Pair