

## List of Abbreviations

<i>Abbreviation</i>	<i>Full form</i>
2D	Two-dimensional
TMDs	Transition Metal Dichalcogenides
JTMDs	Janus Transition Metal Dichalcogenides
LDA	Local Density Approximation
GGA	Generalized Gradient Approximation
mBJ	Modified Becke-Johnson
PBE	Perdew-Burke-Ernzerhof
SCF	Self-Consistent Field
DFT	Density Functional Theory
DFPT	Density Functional Perturbation Theory
BZ	Brillouin zone
BoltzTraP	Boltzmann Transport
QE	Quantum ESPRESSO
ESPRESSO	opEn Source Package for Research in Electronic Structure, Simulation, and Optimization
DOS	Density of States
TDOS	Total Density of States
PDOS	Projected Density of States
SPDOS	Spin Polarized Density of States
HOMO	Highest Occupied Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital
CDD	Charge Density Difference
SCAPS-1D	One Dimensional Solar Cell Capacitance Simulator
CVD	Chemical Vapor Deposition
SOC	Spin Orbit coupling
STEM	Scanning Tunneling Electron Microscopy
AZO	Aluminum doped Zinc Oxide
QE	Quantum Efficiency
vdW	Van der Waals
VBM	Valence Band Maximum
CBM	Conduction Band Minimum
VB	Valence Band
CB	Conduction Band
TCO	Transparent Conducting Oxide
PV	Photovoltaic
CTC	Cumulative lattice Thermal Conductivity

