Explanations on the input and output data

For training of neural network for perovskite solar cells

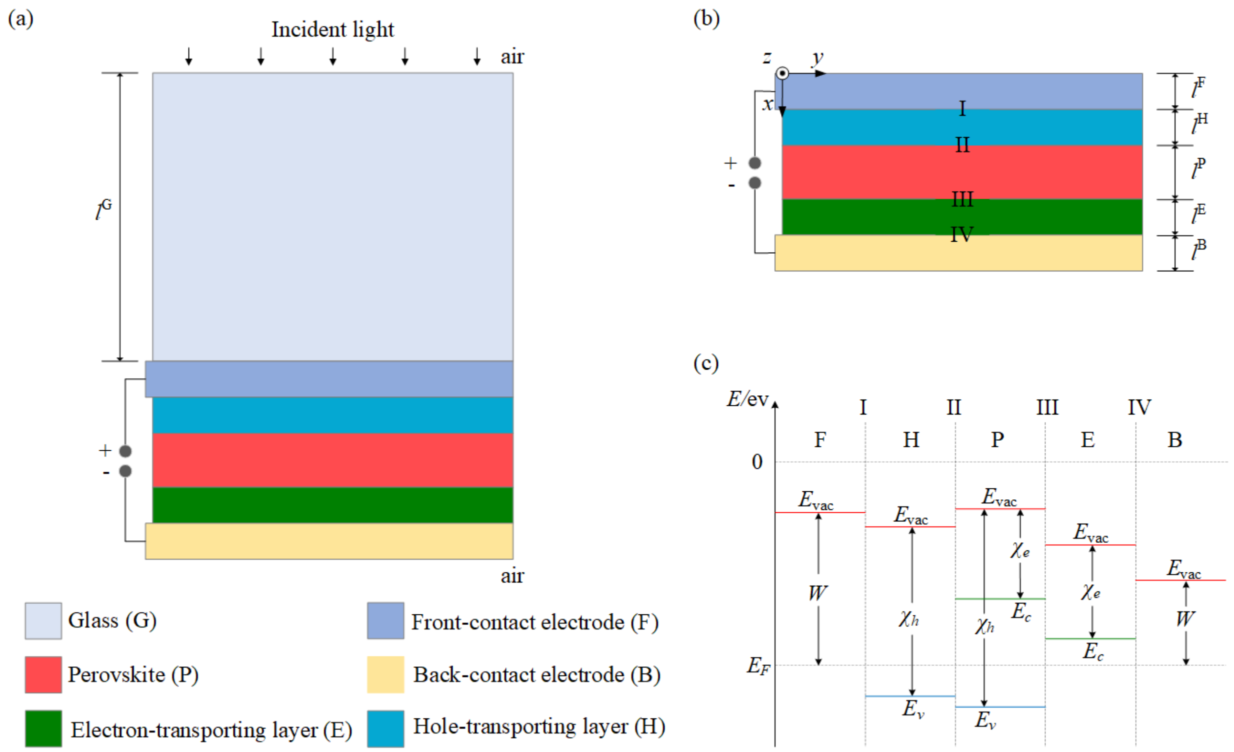

Figure 1: Schematics of (a) a p-i-n perovskite solar cell; (b) the five layers without glass in the perovskite solar cell; and (c) the corresponding energy band diagram.

Table 1: Table headers in the data for training, their corresponding symbols, meanings and units.

Table headers in data (.txt) file	Symbols	Explanations	Units
**Inputs*			
LH	l^{H}	H layer thickness	nm
LP	l^{P}	P layer thickness	nm
LE	l^{E}	E layer thickness	nm
muHh	μ_h^{H}	Hole mobility in H	$\mathrm{m^2\ V^{-1}\ s^{-1}}$
muPh	μ_h^{P}	Hole mobility in P	$\mathrm{m^2\ V^{-1}\ s^{-1}}$
muPe	μ_e^{P}	Electron mobility in P	$\mathrm{m^2\ V^{-1}\ s^{-1}}$
muEe	μ_e^{E}	Electron mobility in E	$\mathrm{m^2\ V^{-1}\ s^{-1}}$
NvH	N_v^{H}	Valance band density of state in H	$\mathrm{m^{-3}}$
NcH	N_c^{H}	Conduction band density of state in H	$\mathrm{m^{-3}}$
NvE	N_v^{E}	Valance band density of state in E	$\mathrm{m^{-3}}$
NcE	N_c^{E}	Conduction band density of state in E	$\mathrm{m^{-3}}$
NvP	N_v^{P}	Valance band density of state in P	$\mathrm{m^{-3}}$
NcP	N_c^{P}	Conduction band density of state in P	$\mathrm{m^{-3}}$
chiHh	χ_h^{H}	Hole ionization potential in H	eV
chiHe	χ_e^{H}	Electron affinity in H	eV
chiPh	χ_h^{P}	Hole ionization potential in P	eV

chiPe	χ_e^{P}	Electron affinity in P	eV
chiEh	χ_h^{E}	Hole ionization potential in E	eV
chiEe	χ_e^{E}	Electron affinity in E	eV
Wlm	W_{B}	Work function of B	eV
Whm	W_{F}	Work function of F	eV
epsH	ε^{H}	Relative permittivity in H	-
epsP	ε^{P}	Relative permittivity in P	-
epsE	ε^{E}	Relative permittivity in E	-
Gavg	G_{avg}	Average charge carrier generation rate in P	$\mathrm{m}^{-3}\ \mathrm{s}^{-1}$
Aug	$A_{(e,h)}$	Auger recombination coefficient in P	$\mathrm{m}^{6}\ \mathrm{s}^{-1}$
Brad	B_{rad}	Radiative recombination coefficient in P	$\mathrm{m}^{3}\ \mathrm{s}^{-1}$
Taue	τ_e	Electron lifetime in P	s
Tauh	τ_h	Hole lifetime in P	s
vII	v_{II}	Interface recombination velocity at II	$\mathrm{m}^{4}\ \mathrm{s}^{-1}$
vIII	v_{III}	Interface recombination velocity at III	$\mathrm{m}^{4}\ \mathrm{s}^{-1}$
**Outputs*			
isc	i_{sc}	Short-circuit current density	$\mathrm{A\ m}^{-1}$
Voc	V_{oc}	Open-circuit voltage	V
FF	$\mathfrak{F}$	Fill factor	-
PCE	η	Power conversion efficiency	-
i_Rrad_MPP	i_{rad}^{MPP}	Loss due to radiative recombination at maximum power point	$\mathrm{A\ m}^{-1}$
i_Rsrh_MPP	i_{srh}^{MPP}	Loss due to Shockley-Read-Hall recombination at maximum power point	$\mathrm{A\ m}^{-1}$
i_Raug_MPP	i_{aug}^{MPP}	Loss due to Auger recombination at maximum power point	$\mathrm{A\ m}^{-1}$
i_RII_MPP	i_{II}^{MPP}	Loss due to interface recombination at II at maximum power point	$\mathrm{A\ m}^{-1}$
i_RIII_MPP	i_{III}^{MPP}	Loss due to interface recombination at III at maximum power point	$\mathrm{A\ m}^{-1}$
i_Rrad_OC	i_{rad}^{OC}	Loss due to radiative recombination at open circuit	$\mathrm{A\ m}^{-1}$
i_Rsrh_OC	i_{srh}^{OC}	Loss due to Shockley-Read-Hall recombination at open circuit	$\mathrm{A\ m}^{-1}$
i_Raug_OC	i_{aug}^{OC}	Loss due to Auger recombination at open circuit	$\mathrm{A\ m}^{-1}$
i_RII_OC	i_{II}^{OC}	Loss due to interface recombination at II at open circuit	$\mathrm{A\ m}^{-1}$
i_RIII_OC	i_{III}^{OC}	Loss due to interface recombination at III at open circuit	$\mathrm{A\ m}^{-1}$
i_Rrad_SC	i_{rad}^{SC}	Loss due to radiative recombination at short circuit	$\mathrm{A\ m}^{-1}$
i_Rsrh_SC	i_{srh}^{SC}	Loss due to Shockley-Read-Hall recombination at short circuit	$\mathrm{A\ m}^{-1}$
i_Raug_SC	i_{aug}^{SC}	Loss due to Auger recombination at short circuit	$\mathrm{A\ m}^{-1}$
i_RII_SC	i_{II}^{SC}	Loss due to interface recombination at II at short circuit	$\mathrm{A\ m}^{-1}$
i_RIII_SC	i_{III}^{SC}	Loss due to interface recombination at III at short circuit	$\mathrm{A\ m}^{-1}$

*The inputs and outputs can be selective. They are also not fixed; for examples:

1) Outputs can be either the cell performances, namely the isc, Voc, FF and PCE, or the recombination losses

2) Information from i-V curves can be the inputs as well?