

## Supporting Information

# Machine Learning Assisted Screening of the Effective Passivation Material for Perovskite Solar Cells with P-I-N Type

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## Data collection and preprocessing:

We collected a total of 95 sets of data based on the passivation material for passivating the perovskite/ETL interface of perovskite solar cells with p-i-n type. Each group of data includes photovoltaic parameters of the device (PCE,  $V_{oc}$  and  $J_{sc}$ ),  $rA$ ,  $AX$ ,  $PX$ , and Molecular SMILES code as shown in **Table S1**. The performance of the device is relatively concentrated, therefore the prediction accuracy in these segments is high.

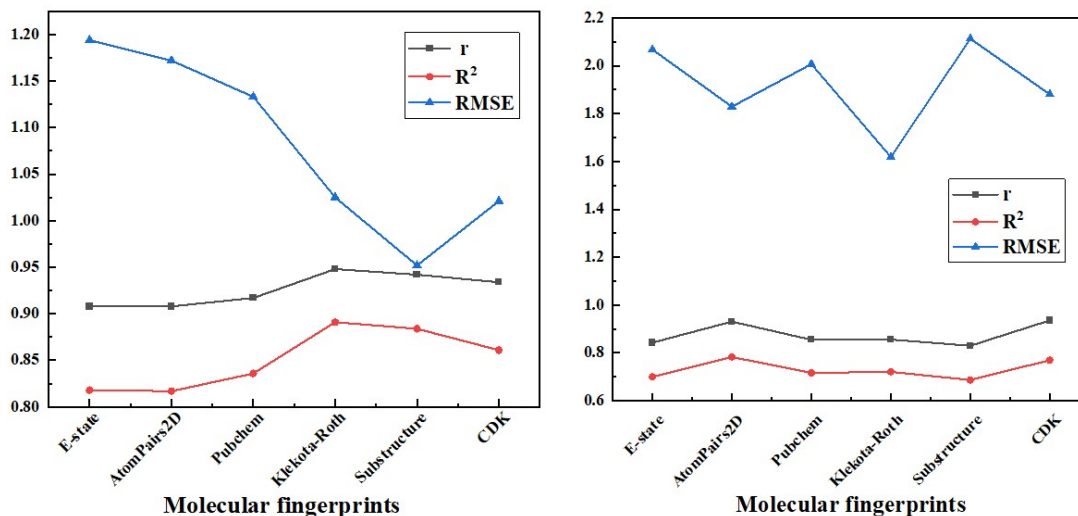


Fig. S1 Evaluation index for six types of the molecular fingerprints with RF model

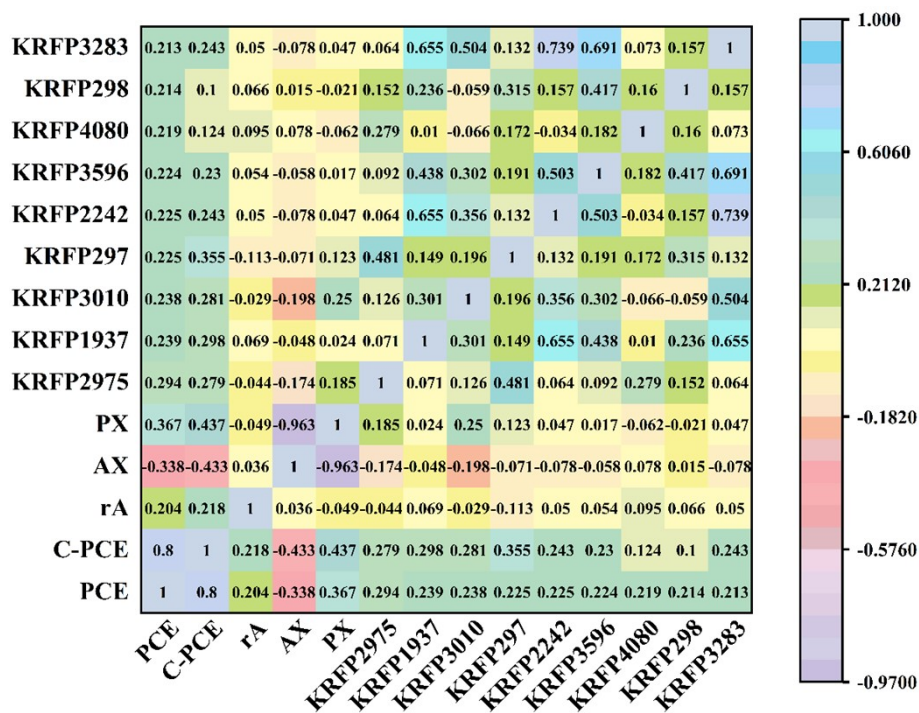


Fig. S2 Correlation matrix between the 13 input features and the PCE. The values are the

Pearson correlation coefficient, and the sign ( $\pm$ ) of the value means positive (+) or negative (-) correlation.

**Model performance evaluation:**

Using the coefficient of determination ( $R^2$ ), the root means square error (RMSE) and Pearson's coefficient ( $r$ ) judge the pros and cons of the algorithm. The calculation formulas are shown in (1) (2) and (3).

$$R^2 = \frac{\left[ \sum_{i=1}^n (x_i - \hat{x})(x'_i - \hat{x}') \right]}{\sum_{i=1}^n (x_i - \hat{x})^2 \cdot \sum_{i=1}^n (x'_i - \hat{x}')^2} \quad (1)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (x'_i - x_i)^2}{n}} \quad (2)$$

$$r = \frac{\sum_{i=1}^n (x_i - \hat{x})(x'_i - \hat{x}')}{\sqrt{\sum_{i=1}^n (x_i - \hat{x})^2} \sqrt{\sum_{i=1}^n (x'_i - \hat{x}')^2}} \quad (3)$$

where  $n$  is the total number of data;  $x_i$  and  $x'_i$  represent the original and predicted values, respectively;  $\hat{x}$  and  $\hat{x}'$  stand for the average of the original and predicted values, respectively. More importantly  $r$ ,  $R^2$ , and RMSE in each algorithm is measured 5 times and the average is used to increase the reliability of algorithm.

**Machine learning settings:**

The algorithm network is all completed by python. After reading the data with pandas, the data set is divided into training set and test set, normalized and standardized. According to the characteristics of the data, the Scikit Learn class is called to initially obtain random forest (RF), K-nearest neighbors (KNN), support vector machine (SVM), extreme gradient boosting (XGBoost), and gradient boosting decision tree (GBDT) to establish the algorithm network model. We divide the data set based on 7:3, which means the training set with 70% of the data is applied for training to obtain the network model parameters of the five algorithms, and then we use the cross-validation method to evaluate the performance for the network model via the remaining 30% of the data.

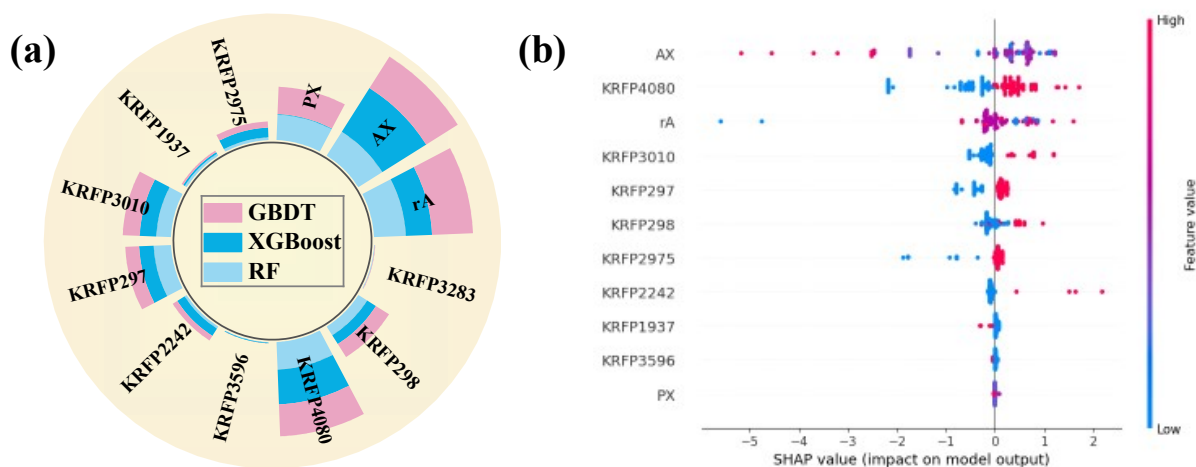


Fig. S3 (a)Polar plots of the feature importance derived from tree-based ML algorithms (GBDT, XGBoost, and RF) and (b)Input feature importance analysis based on XGBoost model.

### Device fabrication:

For the device with ITIC treatment

The indium tin oxide (ITO) substrates with a nominal sheet resistance of 15  $\Omega$ /square were cleaned with detergent and ultrasonicated in special glass lotion, deionized water, and ethanol. The cleaned ITO substrates were dried by nitrogen gas and rested for 15 minutes in the petri dish before UV-ozone treatment. The PEDOT:PSS (Clevios A14083) was filtered through polytetrafluoroethylene (PTFE) filters (0.45 $\mu$ m) prior to the layers fabrication. The PEDOT:PSS was spin-coated onto ITO glass and then thermally annealed at 150  $^{\circ}$ C for 15 min in ambient atmosphere. The substrates with PEDOT:PSS were transferred into a N<sub>2</sub>-filled glove box, where 1.8M CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> solution(the molar ratio of PbI<sub>2</sub> and CH<sub>3</sub>NH<sub>3</sub>I is 1:1 in DMF with 10 wt.% PbCl<sub>2</sub>, and stirred overnight at 65  $^{\circ}$ C. ) was applied onto the ITO/PEDOT:PSS substrates by one spin-coating step at 7500 rpm for 25s. After about 3.5s of the spin-coating, 400  $\mu$ L chlorobenzene (CB) was quickly dripped onto the rotating substrate. After drying the substrate at 100  $^{\circ}$ C for 5 min, phenyl-C61-butyric acid methyl ester (PC<sub>61</sub>BM) solution (30 mg/mL<sup>-1</sup> in CB) was deposited onto the perovskite films. Finally, 5 nm of BCP (Luminescence Technology Corp.) and 100 nm of silver (Ag) were thermally evaporated at  $\sim 10^{-7}$  torr to form the contact electrodes. The active area of perovskite devices is about 1.8 mm<sup>2</sup>.

For the device with ITIC-M treatment

All the perovskite solar cells with ITIC-M treatment were fabricated onto indium tin oxide (ITO)-coated glass substrates. The ITO substrates with sheet resistance of 15  $\Omega$ /□ were consecutively cleaned with glass lotion, de-ionized water, and alcohol. The cleaned ITO glass

substrates were dried by nitrogen gas and then were treated by UV-Ozone for 15 min to further clean the substrates and improve the work function. We use modified PEDOT:PSS (m-PEDOT:PSS) as HTL, the m-PEDOT:PSS was prepared by combining 1 ml filtered PEDOT:PSS , 5 ml de-ionized water and 60 mg sodium polystyrenesulfonate (PSS-Na). The m-PEDOT:PSS was deposited onto ITO substrates at 5000 rounds per minute (rpm) for 20s. Then the substrates were dried in air at 150 °C for 10 min. After that, the substrates were transferred into N<sub>2</sub> glove box. To prepare perovskite films, the MAPbI<sub>3</sub>Cl<sub>3-x</sub> precursor solution(809.25mg of PbI<sub>2</sub>, 20.75mg of PbCl<sub>2</sub>, 300mg of MAI in 1 ml DMF.) was deposited onto m-PEDOT:PSS/ITO substrates at 7000 rpm for 25 s. And the perovskite coated substrates were thermally annealed at 100 °C for 10 min. The PCBM layer was deposited onto the perovskite layer at 1000 rpm for 40 s. Following a layer of BCP with a thickness about 8 nm and a silver (Ag) cathode layer of about 100 nm was deposited under  $4 \times 10^{-4}$  Pa vacuum conditions. The device area is defined by be the overlap of the Ag and ITO electrodes, which is 4 mm<sup>2</sup>.

### **Characterization:**

The current-voltage characteristics of the devices were measured using a Keithley 2400 source meter. The devices were illuminated under 1 sun, AM1.5G from Abet Technologies using a calibrated silicon diode. Steady-state photoluminescence (PL) was measured using a fluorescence spectrometer (Epsilon 3XLE) and Time-resolved photoluminescence spectra (TR-PL) were carried out using a time-correlated single photon counting measurement system with 470

nm excitation wavelength and 770 nm probing wavelength. XRD patterns of the perovskite films were obtained by X-ray diffractometer (XRD) (Ultima IV X-ray diffractometer). AFM measurements were conducted with a Bruker Dimension Fastscan model in tapping mode with reflective probes resonating at 150 kHz frequency. X-ray photoelectron spectroscopy (XPS) measured by Thermo Scientific K-Alpha+ (monochromatic Al Ka, vacuum below  $2 \times 10^{-7}$  mbar, Beam spot 30-400  $\mu\text{m}$  is continuously adjustable with a step size of 5  $\mu\text{m}$ , High performance data acquisition at low power (72 W)). And the surface potential images were performed by MFP-3D Infinity of Asylum Research. The perovskite layer was deposited on Si substrate. There was no buffer layer between Si substrate and perovskite layer. The scanning area and rate were  $2.0 \mu\text{m} \times 2.0 \mu\text{m}$  and 1 HZ, respectively. The lift height for KPFM measurements was 5 nm for all samples. The measurement was carried out under dark condition.

#### **DFT calculation settings and analysis:**

The structural optimization and electronic structure calculations were carried out by Cambridge Serial Total Energy Package (CASTEP) in Materials studio. The generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE) functional was employed. Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm was used for the structural optimization of the model with the following optimization parameters: the calculation was expanded by using the ultrasoft pseudopotential with a cutoff energy of 435 eV, and the total energy was converged to  $2 \times 10^{-5}$  eV.

The structural optimization was optimized until the force tolerance on each atom was smaller than  $0.05\text{eV}\text{\AA}^{-1}$ , the stress tolerance was smaller than 0.1 GPa, and the displacement tolerance was smaller than 0.002 Å. The Monkhorst-Pack grids with the actual spacing of  $0.041\text{\AA}^{-1}$  and SCF tolerance of  $2\times 10^{-6}\text{eV/atom}$  was used in all DFT simulations.

$\text{CH}_3\text{NH}_3\text{PbI}_3$  possesses a cubic structure, with the space group Pm-3m at room temperature. A  $5\times 4\times 1$  super cell and a 15 Å vacuum slab were employed to investigate the adsorption of different additives. The additive was placed on the super cell surface to optimize to convergence. And the solubility of  $\text{PbI}_2$  is generally lower compared to MAI.  $\text{PbI}_2$  with slightly beyond the stoichiometric ratio is used to address this issue. However, this also results in the exposure of  $\text{PbI}_2$  surfaces in  $\text{MAPbI}_3$  perovskite. Therefore, in order to approximate the actual surface state as closely as possible, we established a calcium iron perovskite model based on the  $\text{PbI}_2$  surface for studying the interaction between this surface and ITIC in DFT calculations.

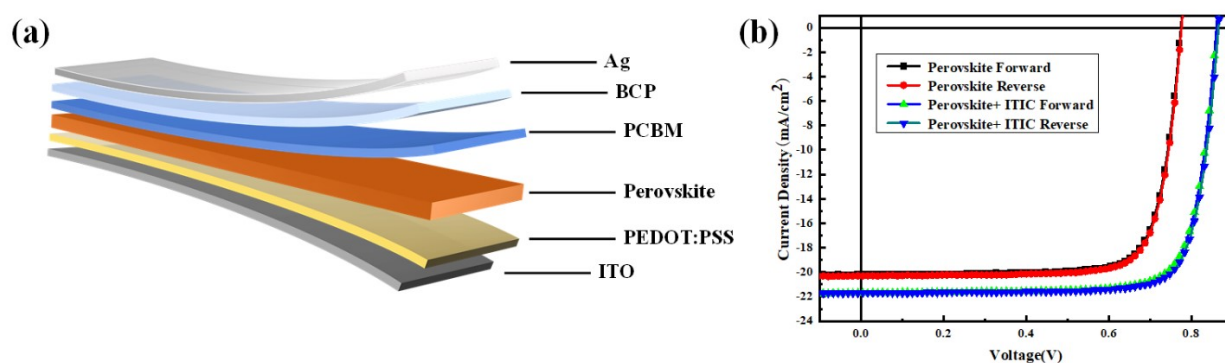


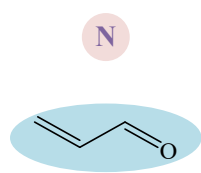
Fig. S4 (a) Structure diagram of PSCs, (b) J-V curves of the devices based on the pristine and treated perovskite films.

Table S1 the device performance of perovskite solar cells with different ITIC concentrations.



| Anti-solvent    | $J_{sc}(\text{mA}/\text{cm}^{-2})$ | $V_{oc}(\text{V})$ | FF(%) | PCE(%) |
|-----------------|------------------------------------|--------------------|-------|--------|
| CB              | 18.67                              | 0.82               | 0.80  | 12.24  |
| CB+ITIC(1mg/ml) | 19.03                              | 0.90               | 0.81  | 13.87  |
| CB+ITIC(2mg/ml) | 19.87                              | 0.92               | 0.80  | 14.62  |
| CB+ITIC(4mg/ml) | 17.57                              | 0.92               | 0.82  | 13.25  |

The most relevant fingerprint  
Fragments For PCE



ITIC-M molecule

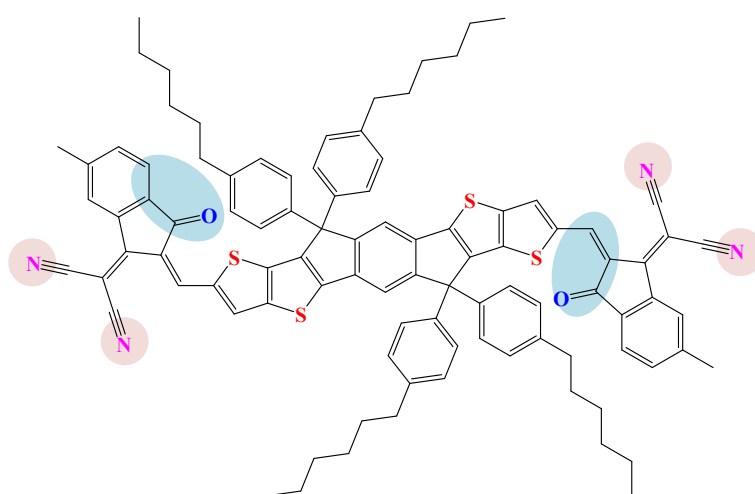


Fig. S5 ITIC-M molecule structure with the effective screened fingerprint fragments.

Table S2 the device performance of perovskite solar cells with different ITIC-M concentrations.

| Anti-solvent      | $J_{sc}(\text{mA}/\text{cm}^{-2})$ | $V_{oc}(\text{V})$ | FF(%) | PCE(%) |
|-------------------|------------------------------------|--------------------|-------|--------|
| CB                | 19.51                              | 0.95               | 0.79  | 14.61  |
| CB+ITIC-M(1mg/ml) | 20.44                              | 1.00               | 0.81  | 16.59  |
| CB+ITIC-M(2mg/ml) | 20.71                              | 1.02               | 0.82  | 17.33  |
| CB+ITIC-M(4mg/ml) | 20.30                              | 0.96               | 0.81  | 15.88  |

Moreover, planar structured perovskite solar cells can be treated as a single junction diode,

it's I-V characteristics can be described by:

$$J = J_{SC} - J_0 \left[ \exp \left( \frac{q(V + JR_s)}{mK_B T} \right) - 1 \right] \quad (4)$$

where  $J$  is the current density flow through the external load,  $J_{SC}$  is the short current density under light,  $J_0$  is the reverse saturation current density,  $q$  is the electron charge,  $V$  is the applied voltage,  $m$  is the ideality factor,  $K_B$  is the Boltzmann constant, and  $T$  is the temperature. When the current flowing through the external circuit is 0, we can obtain  $V_{oc}$  according to Equation (4):

$$V_{OC} = \frac{mK_B T}{q} \ln \left( \frac{J_{SC}}{J_0} + 1 \right) \quad (5)$$

From Equation (5), it can be seen that a higher  $V_{oc}$  corresponds to a lower  $J_0$ . The series resistance ( $R_s$ ) and  $J_0$  of the cells can be calculated according to the diode equation (6) and (7) which come from equation (4):

$$\frac{dV}{dJ} = \frac{mk_B T}{q} (J_{SC} + J)^{-1} + R_s \quad (6)$$

$$\ln (J_{SC} + J) = \frac{q}{mK_B T} (V - J \times R_s) \ln J_0 \quad (7)$$

After the introduction of ITIC and ITIC-M, the  $V_{oc}$  of corresponding devices has been significantly improved, taking the ITIC-M modified device as an example, by linearly fitting the  $\ln(J_{sc}+J)$  vs  $(V+R_s \cdot J)$ , the values of  $J_0$  are calculated for the control and ITIC-M modified device are  $6.51 \times 10^{-8}$  and  $3.90 \times 10^{-9}$  mA/cm<sup>2</sup>, respectively, as shown in Fig. S6. The reduced  $J_0$  will contribute to the improvement of  $V_{oc}$ .

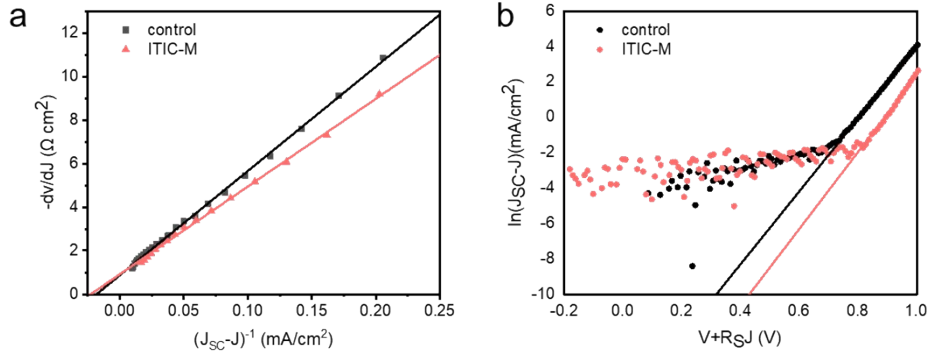


Fig. S6 (a) Plots of  $dV/dJ$  versus  $(J_{sc} + J)^{-1}$  and the linear fitting curves, (b) plots of  $\ln(J_{sc} + J)$  versus  $(V - R_s \cdot J)$  and the linear fitting curves.

$J_0$  reflects the carrier recombination in the perovskite solar cells, according to the scanning electron microscope (SEM) results (Fig. 7Sa-7Sb), the average grain size of ITIC-M modified perovskite film is improved from 349 nm (control film) to 450 nm, as shown in Fig. 7Sc-7Sd, which means there are less grain boundaries in the ITIC-M modified perovskite film. The less grain boundaries will contribute to reduce the non-radiative recombination in the ITIC-M modified perovskite film. On the other hand, the ideality factor  $m$  of control and ITIC-M modified PSCs are calculated according to the slope of curves in Fig. S6(a), which are 1.86 and 1.57, respectively. A perfect solar cell has a  $m$  of unity, if  $m$  approaches 2, charge recombination processes are dominated by non-radiative trap-assisted recombination. An ideality factor  $m$  closer to unity infers that the solar cells operate with less trap-assisted recombination. In the PSCs with ITIC-M, the reduced  $m$  means the less trap-assisted recombination, which is evidence of improvements in  $V_{oc}$ .

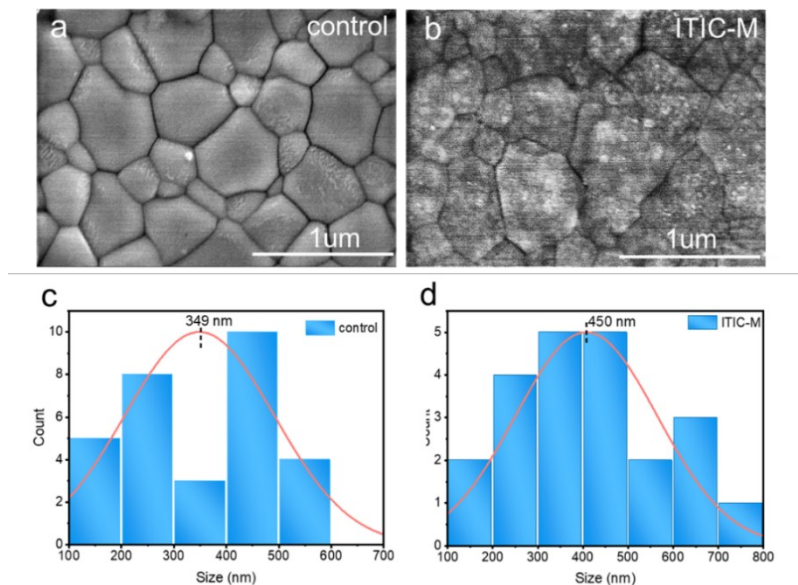


Fig. S7 (a-b) The SEM images of control and ITIC-M modified perovskite films, respectively; (c-d) the distribution of grain size of control and ITIC-M modified perovskite films, respectively.

Table S3 Datasets on the interface passivation at the perovskite/ETL interface of the PSCs

| ID | Passivation materials | Device PCE | Control device PCE | rA    | AX      | PX      | References DOI                |
|----|-----------------------|------------|--------------------|-------|---------|---------|-------------------------------|
| 1  | TPPO                  | 14.9       | 13.7               | 2.7   | 1:3     | 1:3     | 10.1016/j.optmat.2022.112264  |
| 2  | capsaicin             | 21.88      | 19.16              | 2.7   | 0.949:3 | 1.025:3 | 10.1016/j.joule.2020.12.009   |
| 3  | Y6                    | 20.2       | 17.39              | 2.7   | 0.843:3 | 1.079:3 | 10.1021/acsami.1c13447        |
| 4  | 4,4'-Bipyridine       | 16.67      | 15.92              | 2.720 | 1.045:3 | 0.935:3 | 10.1016/j.solener.2019.08.026 |
| 5  | 2,2'-BiPy             | 9.31       | 15.92              | 2.720 | 1.045:3 | 0.935:3 | 10.1016/j.solener.2019.08.026 |
| 6  | BCP                   | 13.11      | 7.05               | 2.7   | 1:3     | 1:3     | 10.1109/JPHOTOV.2017.2651108  |
| 7  | PFNOX                 | 14         | 11.4               | 2.7   | 1.8:3   | 0.6:3   | 10.1002/adv.201500353         |
| 8  | C3AI                  | 20.3       | 17.7               | 2.7   | 1:3     | 1:3     | 10.1016/j.dyepig.2021.109385  |
| 9  | C3A                   | 19.6       | 17.7               | 2.7   | 1:3     | 1:3     | 10.1016/j.dyepig.2021.109385  |
| 10 | C4                    | 19.6       | 17.7               | 2.7   | 1:3     | 1:3     | 10.1016/j.dyepig.2021.109385  |
| 11 | PVK                   | 19.65      | 16.54              | 2.7   | 1:3     | 1:3     | 10.1021/acsam.1c00219         |
| 12 | 2-HI-PVK              | 12.88      | 12.23              | 2.7   | 1:3     | 1:3     | 10.1021/acsam.9b00757         |
| 13 | 4-HI-PVK              | 13.76      | 12.23              | 2.7   | 1:3     | 1:3     | 10.1021/acsam.9b00757         |
| 14 | P4VP                  | 20.02      | 17.46              | 2.7   | 1:3     | 1:3     | 10.1039/C9TC06578D            |

|    |                   |       |       |       |         |         |                              |
|----|-------------------|-------|-------|-------|---------|---------|------------------------------|
| 15 | PS-PAN            | 22.02 | 18.18 | 2.742 | 0.95:3  | 1.059:3 | 10.1016/j.nanoen.2020.105731 |
| 16 | PHMT              | 21.11 | 18.11 | 2.7   | 1:3     | 1:3     | 10.1016/j.jechem.2020.12.035 |
| 17 | ETMT              | 19.36 | 18.11 | 2.7   | 1:3     | 1:3     | 10.1016/j.jechem.2020.12.035 |
| 18 | PRMT              | 18.57 | 18.11 | 2.7   | 1:3     | 1:3     | 10.1016/j.jechem.2020.12.035 |
| 19 | DPSI              | 21.1  | 19.1  | 2.777 | 1:3     | 1:3     | 10.1002/adma.201803428       |
| 20 | TMTA              | 20.22 | 19.08 | 2.7   | 1:3     | 1:3     | 10.1038/s41467-018-06204-2   |
| 21 | PU                | 18.7  | 16.4  | 2.7   | 1:3     | 1:3     | 10.1002/adfm.201703061       |
| 22 | SP1               | 18.75 | 18.19 | 2.7   | 1:3     | 1:3     | 10.1002/aenm.201803766       |
| 23 | SP2               | 19.27 | 18.19 | 2.7   | 1:3     | 1:3     | 10.1002/aenm.201803766       |
| 24 | SP3               | 20.43 | 18.19 | 2.7   | 1:3     | 1:3     | 10.1002/aenm.201803766       |
| 25 | PBTI              | 20.67 | 18.89 | 2.712 | 0.989:3 | 1.005:3 | 10.1002/adfm.201808855       |
| 26 | PEA               | 20.9  | 20.5  | 2.712 | 0.989:3 | 1.005:3 | 10.1038/s41560-019-0538-4    |
| 27 | BA                | 20.8  | 20.5  | 2.712 | 0.989:3 | 1.005:3 | 10.1038/s41560-019-0538-4    |
| 28 | Oam               | 23    | 20.5  | 2.712 | 0.989:3 | 1.005:3 | 10.1038/s41560-019-0538-4    |
| 29 | BMIMBF4           | 19.8  | 18.5  | 2.727 | 0.953:3 | 1.049:3 | 10.1038/s41586-019-1357-2    |
| 30 | F-PDI             | 18.28 | 15.37 | 2.7   | 1:3     | 1:3     | 10.1002/aenm.201900198       |
| 31 | PFN-2TNDI         | 16.7  | 12.9  | 2.7   | 1.8:3   | 0.6:3   | 10.1002/aenm.201501534       |
| 32 | HATNASOC7-Cs      | 17.62 | 15.91 | 2.7   | 0.949:3 | 1.025:3 | 10.1002/anie.201604399       |
| 33 | HATNASO2C7-<br>Cs | 14.42 | 15.91 | 2.7   | 0.949:3 | 1.025:3 | 10.1002/anie.201604399       |
| 34 | HATNAS3C4         | 11.59 | 15.91 | 2.7   | 0.949:3 | 1.025:3 | 10.1002/anie.201604399       |
| 35 | HATNAS3C7         | 13.49 | 15.91 | 2.7   | 0.949:3 | 1.025:3 | 10.1002/anie.201604399       |
| 36 | HATNAS3C7-<br>C3h | 13.38 | 15.91 | 2.7   | 0.949:3 | 1.025:3 | 10.1002/anie.201604399       |
| 37 | HATNAS3C7-C3      | 13.95 | 15.91 | 2.7   | 0.949:3 | 1.025:3 | 10.1002/anie.201604399       |
| 38 | ITIC-Th           | 22.87 | 21.85 | 2.716 | 0.989:3 | 1.005:3 | 10.1002/adma.202202100       |
| 39 | IT-Cl             | 23.74 | 21.85 | 2.716 | 0.989:3 | 1.005:3 | 10.1002/adma.202202100       |
| 40 | NAP               | 13.4  | 10.3  | 2.7   | 1.5:3   | 0.75:3  | 10.1016/j.jsci.2018.11.003   |
| 41 | EVA               | 19.01 | 17.15 | 2.674 | 0.871:3 | 1.112:3 | 10.1002/adfm.201902629       |
| 42 | AIA               | 15.7  | 13.6  | 2.7   | 1:3     | 1:3     | 10.1002/adsu.202000078       |
| 43 | HIA               | 17.29 | 13.6  | 2.7   | 1:3     | 1:3     | 10.1002/adsu.202000078       |
| 44 | CA                | 19.06 | 13.6  | 2.7   | 1:3     | 1:3     | 10.1002/adsu.202000078       |
| 45 | SubPc             | 13.6  | 9.96  | 2.7   | 1.8:3   | 0.6:3   | 10.1109/JPHOT.2016.2608619   |
| 46 | PNDI-2T           | 21.13 | 19    | 2.7   | 1:3     | 1:3     | 10.1002/solr.202100236       |
| 47 | thiazole          | 17.98 | 14.34 | 2.7   | 1:3     | 1:3     | 10.1021/acsami.8b16124       |
| 48 | PEGDA             | 21.03 | 18.73 | 2.7   | 1:3     | 1:3     | 10.1021/acsami.0c11468       |
| 49 | PLL               | 19.45 | 16.72 | 2.7   | 1:3     | 1:3     | 10.1016/j.jechem.2020.05.040 |
| 50 | PVA               | 17.28 | 16.46 | 2.7   | 1:3     | 1:3     | 10.1021/acsami.1c08539       |
| 51 | PMA               | 19.05 | 16.46 | 2.7   | 1:3     | 1:3     | 10.1021/acsami.1c08539       |

|    |             |       |       |       |         |         |                              |
|----|-------------|-------|-------|-------|---------|---------|------------------------------|
| 52 | PAA         | 20.29 | 16.46 | 2.7   | 1:3     | 1:3     | 10.1021/acsami.1c08539       |
| 53 | 2FEABr      | 21.06 | 19.44 | 2.7   | 0.949:3 | 1.025:3 | 10.1007/s40820-022-00854-0   |
| 54 | AIBN        | 19.56 | 16.92 | 2.7   | 1:3     | 1:3     | 10.1002/solr.202200238       |
| 55 | AIBME       | 19.69 | 16.92 | 2.7   | 1:3     | 1:3     | 10.1002/solr.202200238       |
| 56 | ACVA        | 19.21 | 16.92 | 2.7   | 1:3     | 1:3     | 10.1002/solr.202200238       |
| 57 | BDAI2       | 23.1  | 20.8  | 2.643 | 0.85:3  | 1.15:3  | 10.1002/adfm.202205009       |
| 58 | PDAI2       | 22.2  | 20.8  | 2.643 | 0.85:3  | 1.15:3  | 10.1002/adfm.202205009       |
| 59 | TFBA        | 20.39 | 19.09 | 2.574 | 1:3     | 1:3     | 10.1002/inf2.12307           |
| 60 | HA          | 19.5  | 18.4  | 2.612 | 0.824:3 | 1.176:3 | 10.1016/j.nanoen.2022.107193 |
| 61 | BA          | 19.77 | 18.4  | 2.612 | 0.824:3 | 1.176:3 | 10.1016/j.nanoen.2022.107193 |
| 62 | PA          | 20    | 18.4  | 2.612 | 0.824:3 | 1.176:3 | 10.1016/j.nanoen.2022.107193 |
| 63 | PHA         | 20.72 | 18.4  | 2.612 | 0.824:3 | 1.176:3 | 10.1016/j.nanoen.2022.107193 |
| 64 | TEAI        | 19.19 | 18.62 | 2.744 | 0.924:3 | 1.053:3 | 10.1002/ange.202202346       |
| 65 | TEASCN      | 21.26 | 18.62 | 2.744 | 0.924:3 | 1.053:3 | 10.1002/ange.202202346       |
| 66 | QA          | 15.6  | 13.4  | 2.7   | 1:3     | 1:3     | 10.1016/j.cej.2022.135107    |
| 67 | CH3         | 17.91 | 17.49 | 2.744 | 0.824:3 | 1.176:3 | 10.1016/j.apsusc.2021.151740 |
| 68 | CHO         | 18.68 | 17.49 | 2.744 | 0.824:3 | 1.176:3 | 10.1016/j.apsusc.2021.151740 |
| 69 | COCH3       | 18.86 | 17.49 | 2.744 | 0.824:3 | 1.176:3 | 10.1016/j.apsusc.2021.151740 |
| 70 | BHF         | 20.3  | 16.2  | 2.643 | 0.85:3  | 1.15:3  | 10.1002/solr.202200296       |
| 71 | DMAII       | 13.14 | 10.53 | 1.81  | 0.793:3 | 1.103:3 | 10.1021/acsami.1c23637       |
| 72 | BABr        | 20.3  | 18.5  | 2.7   | 1:3     | 1:3     | 10.1039/d2ee00759b           |
| 73 | Trometamol  | 17.91 | 16.25 | 2.7   | 1:3     | 1:3     | 10.1021/acs.jpcclett.2c01089 |
| 74 | HaHc        | 9.18  | 4.75  | 2.79  | 1:3     | 1:3     | 10.1016/j.cej.2021.133745    |
| 75 | PEAI        | 19.58 | 17.07 | 2.772 | 1:3     | 1:3     | 10.1002/adma.202110241       |
| 76 | EDAI        | 20.67 | 17.07 | 2.772 | 1:3     | 1:3     | 10.1002/adma.202110241       |
| 77 | PEAI-EDAI   | 22.51 | 17.07 | 2.772 | 1:3     | 1:3     | 10.1002/adma.202110241       |
| 78 | TFAA        | 20.1  | 15.08 | 2.7   | 1:3     | 1:3     | 10.1021/acsam.1c02984        |
| 79 | FPA         | 21.28 | 17.87 | 2.7   | 1:3     | 1:3     | 10.1002/solr.202101101       |
| 80 | 2-TPAA      | 14.23 | 12.94 | 1.81  | 1:3     | 1:3     | 10.1016/j.cej.2022.136242    |
| 81 | KBF4        | 23.04 | 21.13 | 2.604 | 0.888:3 | 1.135:3 | 10.1002/adfm.202204880       |
| 82 | dtdn        | 18.34 | 16.76 | 2.7   | 1:3     | 1:3     | 10.1039/d1se01892b           |
| 83 | coumarin343 | 19.8  | 18    | 2.643 | 0.85:3  | 1.15:3  | 10.1016/j.nanoen.2022.106935 |
| 84 | 3-HBA       | 23.25 | 21.56 | 2.741 | 0.917:3 | 1.065:3 | 10.1002/ange.202206914       |
| 85 | SA          | 19.48 | 18.32 | 2.7   | 1:3     | 1:3     | 10.1016/j.apsusc.2022.152670 |
| 86 | PTA         | 20.3  | 18.32 | 2.7   | 1:3     | 1:3     | 10.1016/j.apsusc.2022.152670 |
| 87 | GuaBF4      | 20.87 | 18.09 | 2.7   | 1:3     | 1:3     | 10.1016/j.solmat.2022.111682 |
| 88 | BCP-3N      | 20.9  | 18.7  | 2.729 | 1.151:3 | 0.924:3 | 10.1002/solr.202200559       |
| 89 | BCP-Oam     | 17.3  | 18.7  | 2.729 | 1.151:3 | 0.924:3 | 10.1002/solr.202200559       |
| 90 | BCP-3N-I    | 14.8  | 18.7  | 2.729 | 1.151:3 | 0.924:3 | 10.1002/solr.202200559       |

|    |             |       |       |       |         |         |                            |
|----|-------------|-------|-------|-------|---------|---------|----------------------------|
| 91 | DMAI-TFMPHC | 21.4  | 18.3  | 2.755 | 0.941:3 | 1.039:3 | 10.1016/j.ccej.2022.135974 |
| 92 | DMAI        | 20.7  | 18.3  | 2.755 | 0.941:3 | 1.039:3 | 10.1016/j.ccej.2022.135974 |
| 93 | TFMPHC      | 19.9  | 18.3  | 2.755 | 0.941:3 | 1.039:3 | 10.1016/j.ccej.2022.135974 |
| 94 | COTIC-4F    | 20.69 | 20.52 | 2.736 | 0.935:3 | 1.052:3 | 10.1002/aenm.202200005     |
| 95 | PTB7-Th     | 21.4  | 20.52 | 2.736 | 0.935:3 | 1.052:3 | 10.1002/aenm.202200005     |

The specific code:

```
import numpy as np
import pandas as pd
import shap
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.model_selection import KFold
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import cross_val_score, GridSearchCV
from sklearn import metrics
from pandas import read_csv
import xgboost as xgb
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn.svm import SVR
from sklearn.neighbors import KNeighborsRegressor
from scipy import stats
from sklearn.metrics import mean_squared_error
from sklearn.metrics import r2_score
from matplotlib.pyplot import savefig
#Read data
filename = '.csv'
```

```

data0 = read_csv(filename)

X = data0.iloc[:, :]

y = data0.iloc[:, ]

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=test_size, random_state=10)

scaler = StandardScaler()

scaler.fit(X_train)

X_train_std = scaler.transform(X_train)

X_test_std = scaler.transform(X_test)

#Select model

#XGBoost

param_grid = {'learning_rate': [0.1,0.15,0.35], 'max_depth': [3], 'min_child_weight':
[3,4,5], 'colsample_bytree': [0.8], 'gamma': [0, 0.1, 0.2, 0.3], 'reg_alpha': [0, 0.1, 0.2,
0.3], 'reg_lambda': [1,3,5]}

#GBDT

param_grid = {'n_estimators': [5,10,20,30,40,50,60,70,80,90,100,500], 'max_features':
['auto', 'sqrt'], 'max_depth': range(1,10), 'min_samples_leaf': [1, 2],}

#RF

param_grid = {'n_estimators': [10,20,30,40,50,60,70,80,100,500], 'max_features': ['auto',
'sqrt'], 'max_depth': [3,5,8], 'min_samples_split': [2,3,5], 'min_samples_leaf': [1,2], 'bootstrap':
[True]}

#SVM

param_grid={'kernel':['linear','poly','rbf','sigmoid'], 'degree':[1,2,3], 'gamma':[0.01,0.05,0.1,0.
2,0.5,0.6,0.8], 'C':[0.1,0.2,0.3,0.4,0.5,1], 'epsilon':[0.5,1,2]}

#kNN

param_grid = {'weights': ['uniform'], 'n_neighbors': range(2, 20), 'algorithm':
['ball_tree', 'kd_tree', 'brute']}

```



```
#Fit and predict

best_model = model.best_estimator_

y_train_hat = best_model.predict(X_train_std)
y_test_hat = best_model.predict(X_test_std)

#SHAP

xgb_model = xgb.XGBRegressor(random_state=42)
xgb_model = RandomForestRegressor(random_state=42)
xgb_model = GradientBoostingRegressor(random_state=42)
xgb_model.fit(X_train, Y_train)

shap.initjs()
explainer = shap.TreeExplainer(xgb_model)
shap.initjs()
shap_value = explainer.shap_values(X)
print(shap_value)
shap.summary_plot(shap_value, X)
shap.summary_plot(shap_value, X, plot_type="bar")
abs_shapvalue = abs(shap_value)
shap_average = np.average(abs_shapvalue,axis=0)
print(shap_average)
```