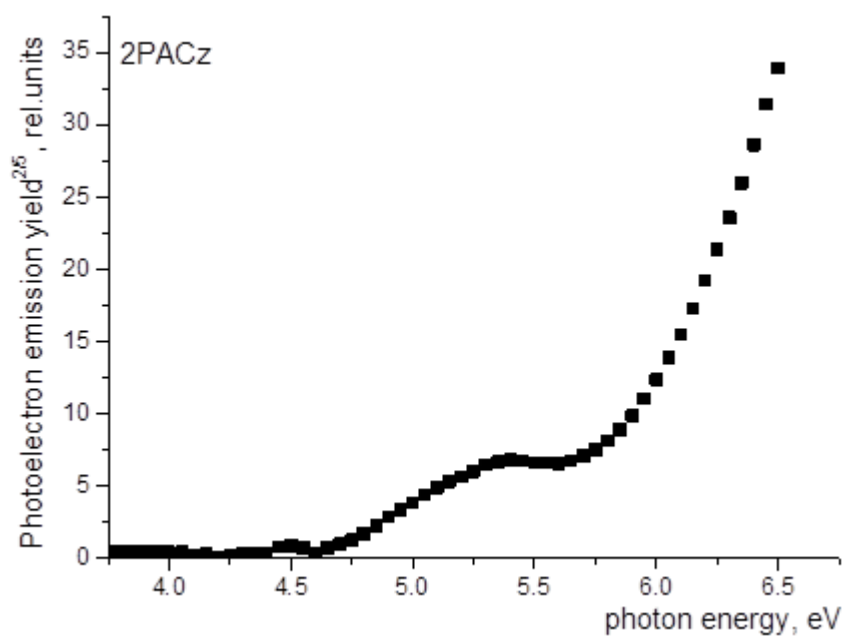
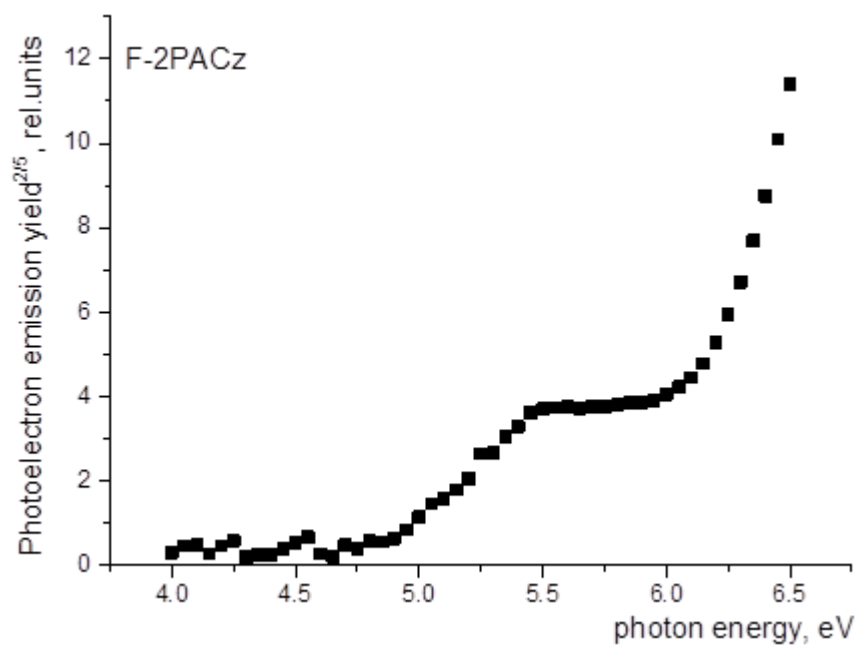
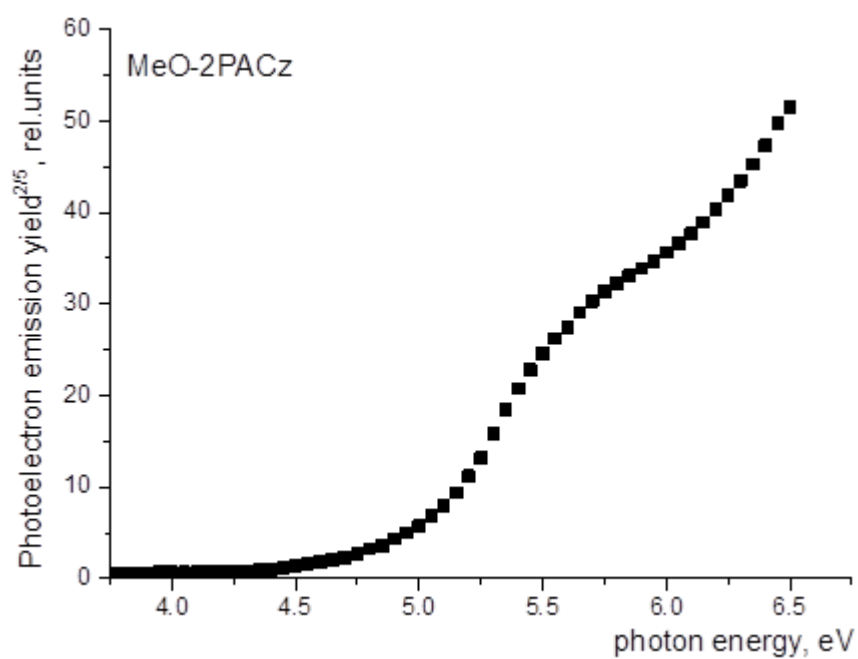


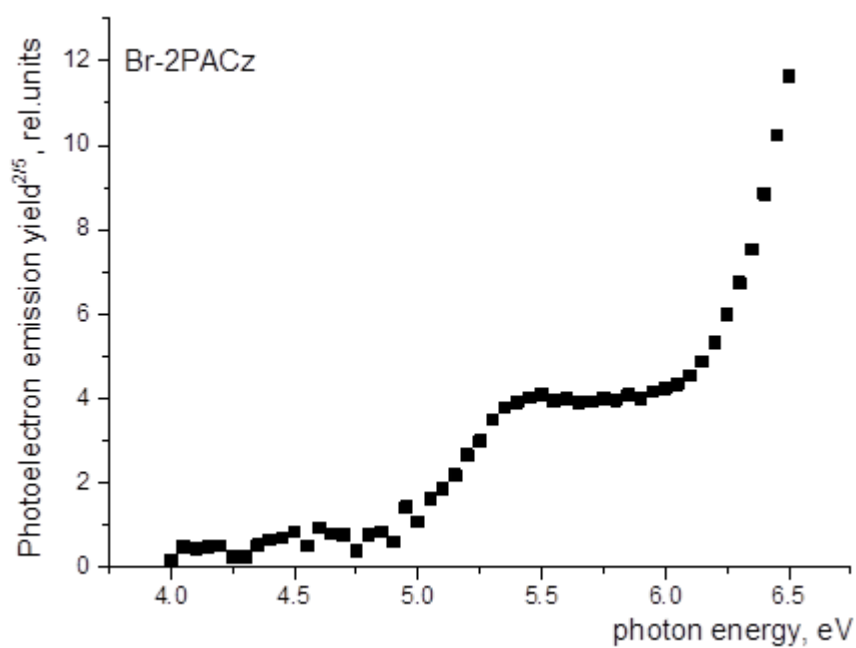
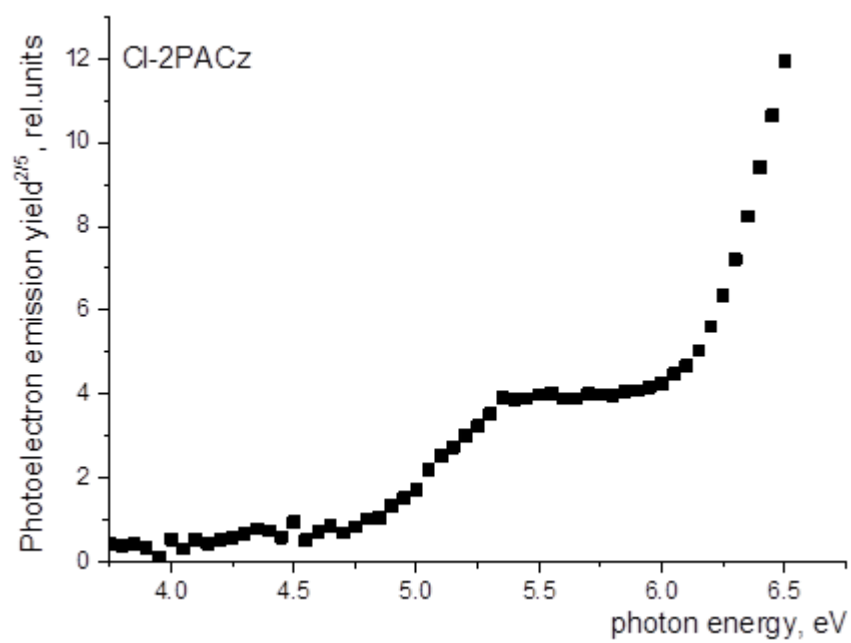
Supplementary Information

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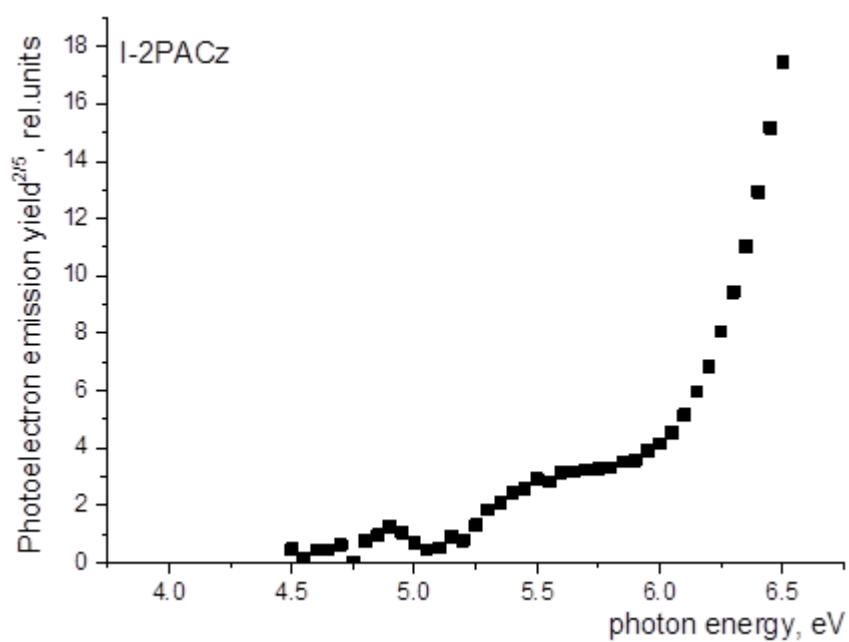
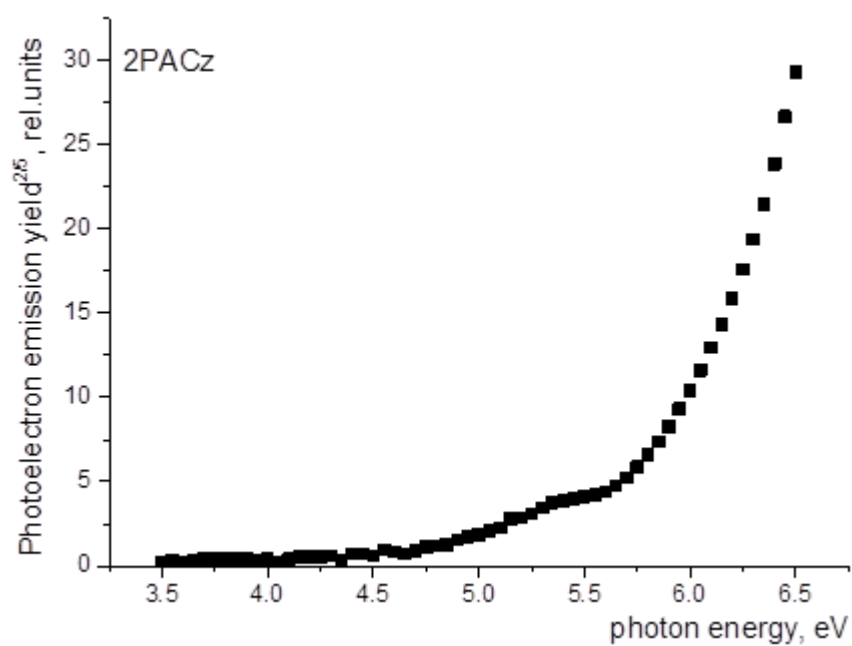
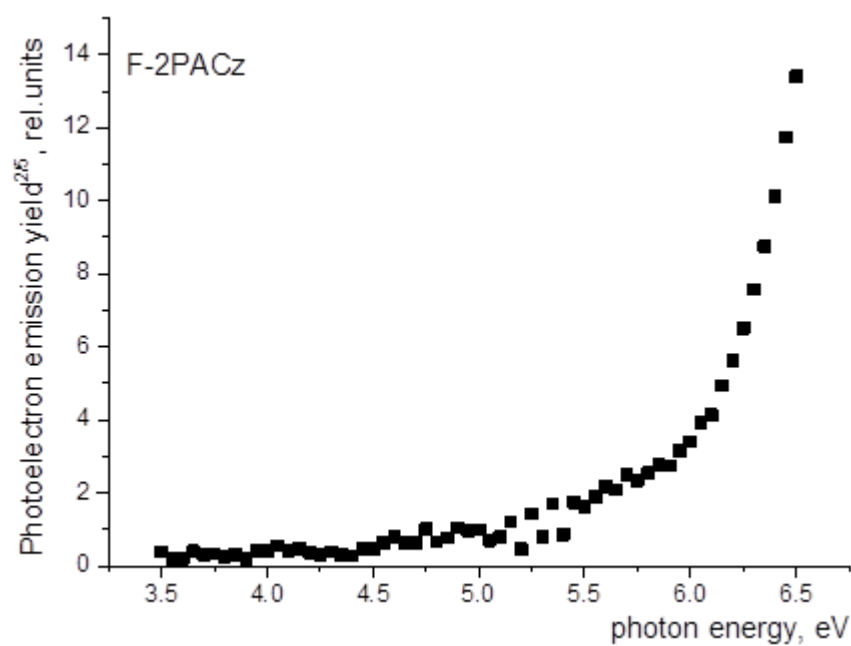
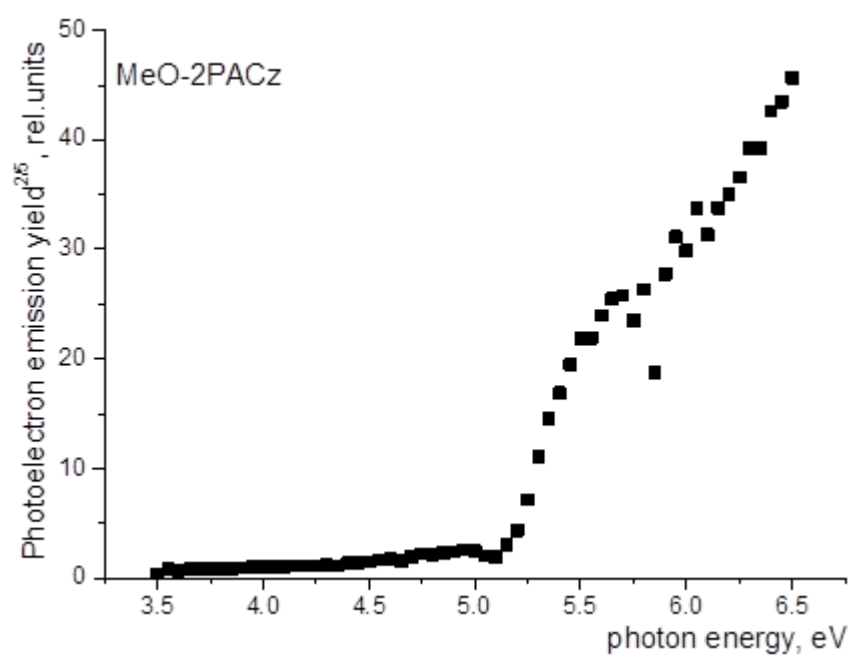
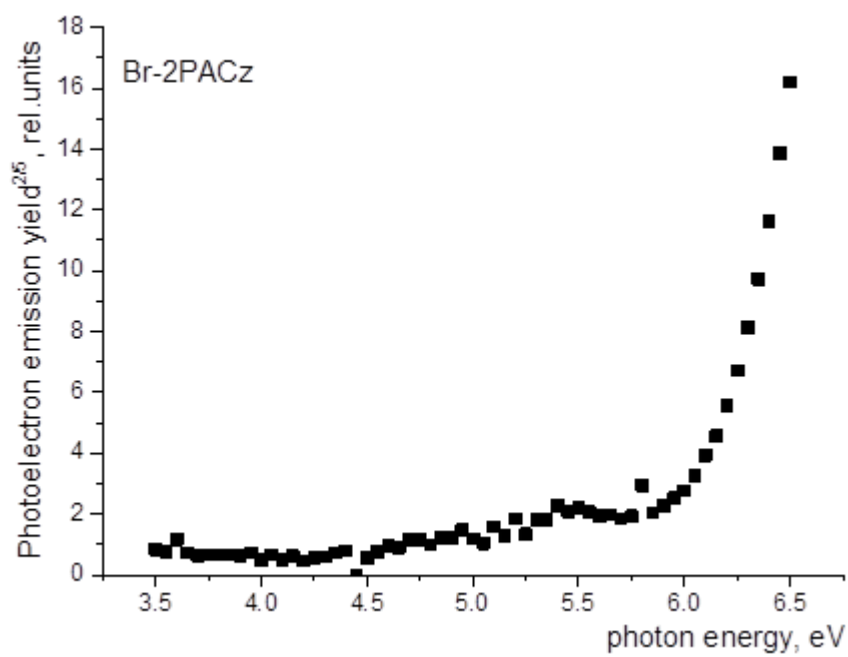
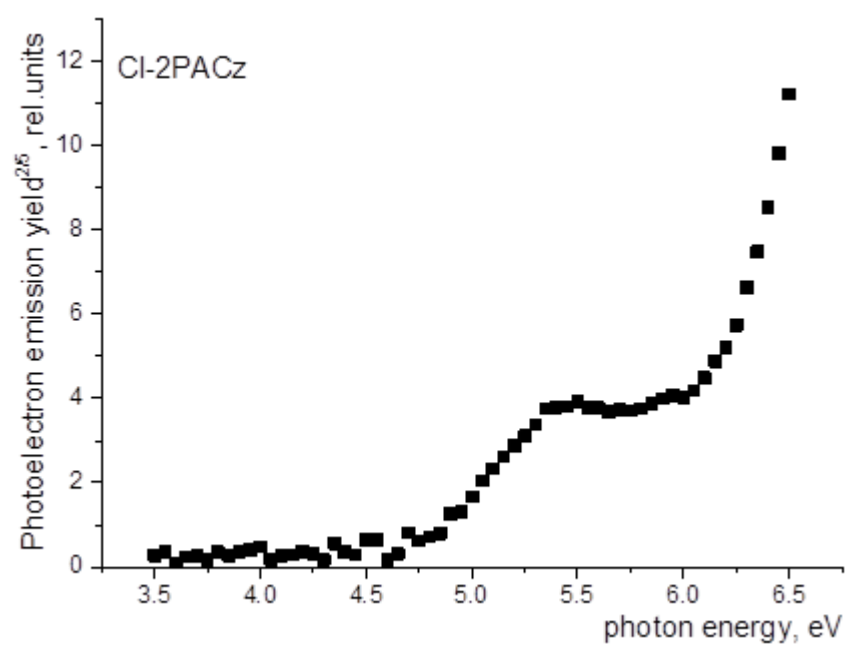


Figure S1. Photoelectron emission yield spectra of SAM films







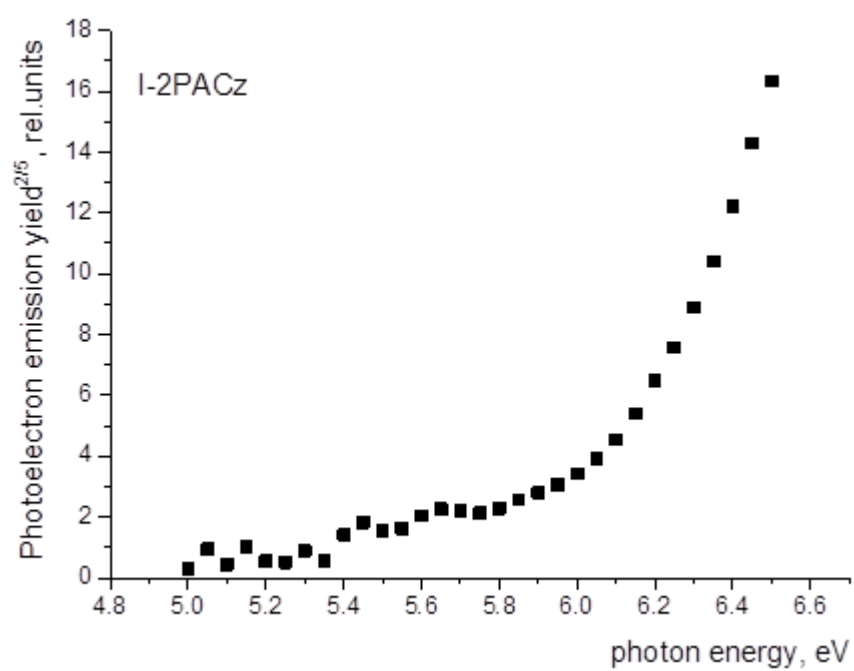
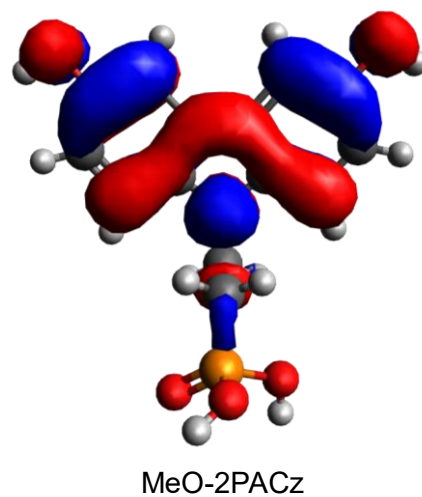
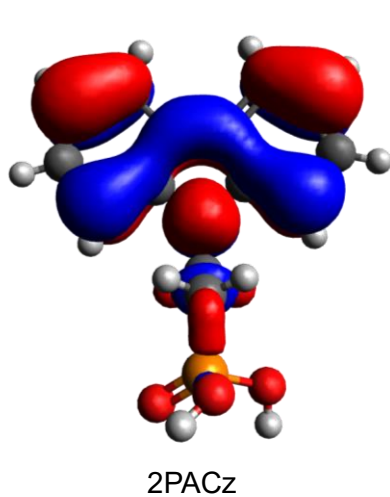


Figure S2. Photoelectron emission yield spectra of bulky samples



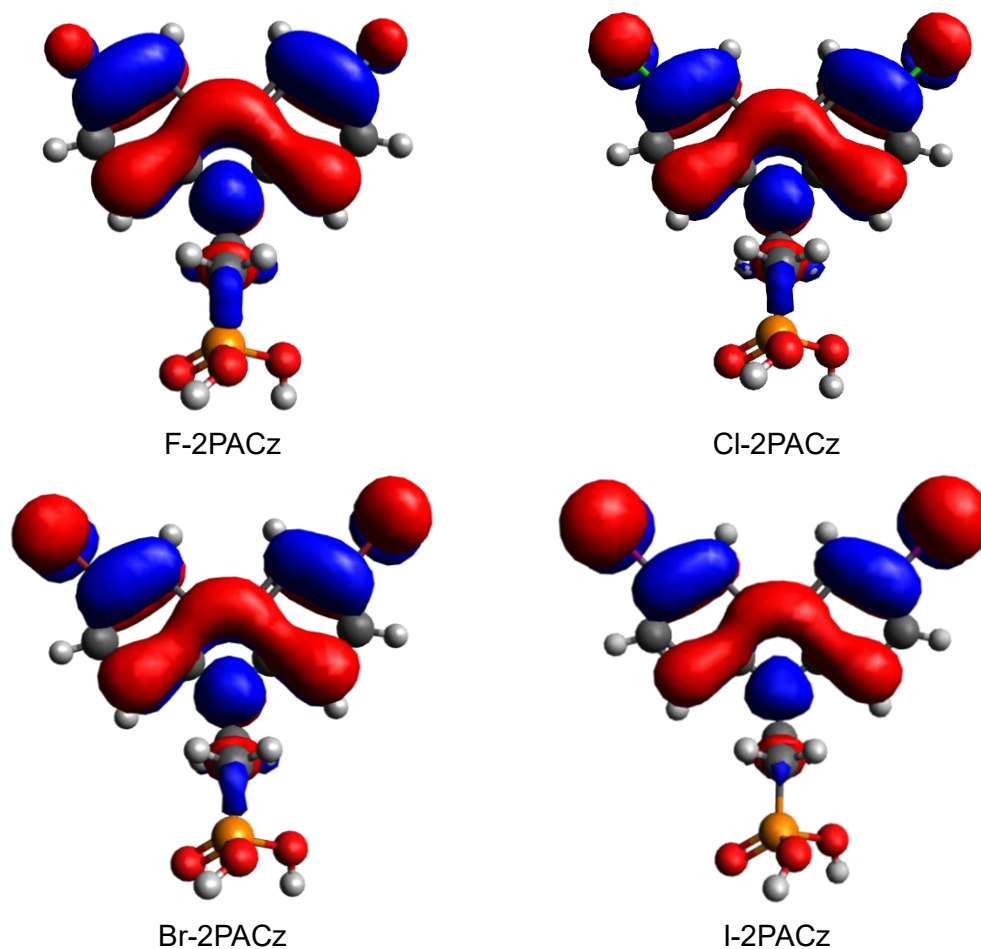


Figure S3. Highest occupied molecular orbital of SAM.

Table S1. Photovoltaic parameters of bulk heterojunction solar cells from references [25-27]. V_{oc} – open circuit voltage, FF – fill factor, J_{sc} – short circuit current, PCE – power conversation efficiency.

SAM	V_{oc} , V	FF, %	J_{sc} , mA/cm^2	PCE, %	References
2PACz	0.845	79.2	26.94	18.03	[1]
MeO-2PACz	0.776	71.3	26.21	14.5	[2]
F-2PACz	0.846	78.2	26.8	17.7	[3]
Cl-2PACz	0.863	79.4	26.96	18.5	[3]
Br-2PACz	0.870	77.9	26.57	18.0	[3]
I-2PACz	0.858	78.8	26.85	18.2	[3]

Correlation coefficient was calculated by the formula:

$$R = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}},$$

where x – ionisation energy value or work function- value, y – solar cells parameter, \bar{x} and \bar{y} – mean values of the parameters.

References

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