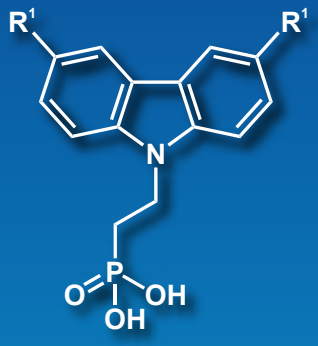
MATERIALS

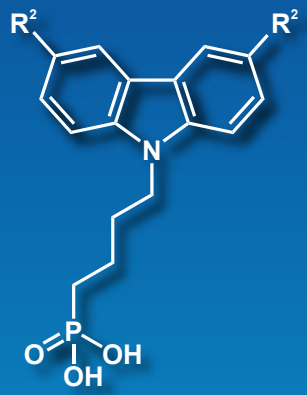
TCI

For Highly Efficient Solar Cells,

Hole-Selective, Self-Assembled Monolayer (SAM)-Forming Agents



2PACz series



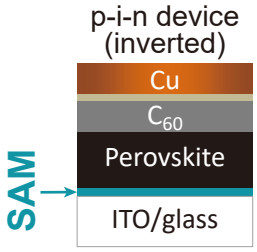
4PACz series

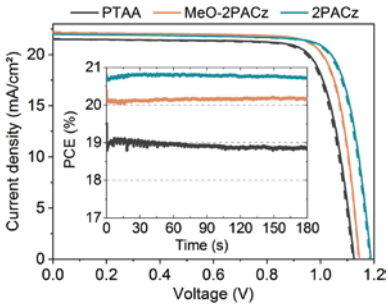
R^1=H	2PACz	500mg	[C3663]
R^1=MeO	MeO-2PACz	500mg	[D5798]
R^1=Me	Me-2PACz	500mg	[M3477]
R^1=Br	Br-2PACz	500mg	[B6391]
R^1=Cl	Cl-2PACz	500mg	[C3914]
R^1=F	F-2PACz	500mg	[F1374]
R^1=I	I-2PACz	500mg	[I1255]
R^2=H	4PACz	500mg	[P2995]
R^2=MeO	MeO-4PACz	500mg	[M3549]
R^2=Me	Me-4PACz	500mg	[M3359]
R^2=Br	Br-4PACz	500mg	[B6445]

Advantages

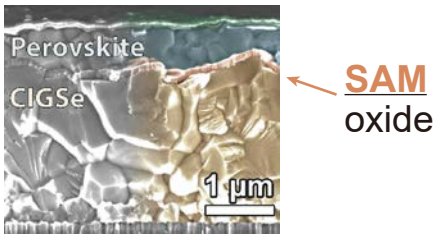
- Enable efficient, versatile and stable solar cell devices without additives, interlayers or dopants
- Self-assembly leads to conformal coverage of oxide surfaces (including textured)
- Simple, scalable and extremely cost-effective processing

Application





Efficiency on 1 cm² = **23.26%**



World-record CIGSe/perovskite tandem enabled by conformal SAM

Stabilized power conversion efficiencies of PSC and OPV with self-assembled monolayer (SAM):

SAM	CsMAFA	MAFA	Co-evaporated $MAPbI_3$	Slot-die coated $MAPbI_3$	CIGSe/CsMAFA tandem	Silicon/CsMAFA tandem	OPV Ternary BHJ
2PACz	20.8%[1)]	21.1%[1)]	-	20.8%[5)]	-	27.36%[3)]	18.03%[4)]
MeO-2PACz	20.2%[1)]	21.1%[1)]	20.6%[2)]	-	23.26%, certified[1)]	28.60%[3)]	-
Me-4PACz	20.8%[3)]	-	-	-	24.16% certified[6)]	29.15%, certified[3)]	-
Br-2PACz	-	-	-	-	-	-	18.4%[7)]

(CsMAFA = $Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})_3$, MAFA = $MA_{0.05}FA_{0.95}Pb(I_{0.95}Br_{0.05})_3$,
Cs = cesium, MA = methylammonium, FA = formamidinium, CIGSe = copper indium gallium selenide)

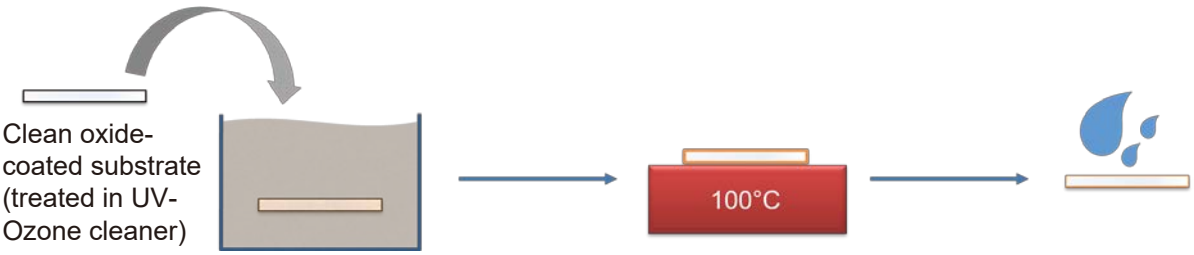
* These data are from References below:
1) A. Al-Ashouri, A. Magomedov, V. Getautis, S. Albrecht, *et al.*, *Energy Environ. Sci.* **2019**, *12*, 3356. https://doi.org/10.1039/C9EE02268F
2) M. Roß, S. Albrecht, *et al.*, *ACS Appl. Mater. Interfaces* **2020**, *12*, 39261. https://doi.org/10.1021/acsami.0c10898
3) A. Al-Ashouri, A. Magomedov, V. Getautis, S. Albrecht, *et al.*, *Science* **2020**, *370*, 1300. https://doi.org/10.1126/science.abd4016
4) Y. Firdaus, T. D. Anthopoulos, *et al.*, *ACS Energy Lett.* **2020**, *5*, 2935. https://doi.org/10.1021/acsenergylett.0c01421
5) J. Li, A. Abate, E. Unger, *et al.*, *Adv. Energy Mater.* **2021**, *11*, 2003460. https://doi.org/10.1002/aenm.202003460
6) NREL Best Research-Cell Efficiency Chart https://www.nrel.gov/pv/cell-efficiency.html
7) Y. Lin, A. Magomedov, V. Getautis, T. D. Anthopoulos, *et al.*, *ChemSusChem* **2021**, *14*, 3569. https://doi.org/10.1002/cssc.202100707

For Highly Efficient Solar Cells, Hole-Selective, Self-Assembled Monolayer (SAM)-Forming Agents

Processing

Method 1: Dip coating

suitable for large-area coating and textured substrates



Clean oxide-coated substrate (treated in UV-Ozone cleaner)

Immersion into SAM forming agent solution (0.5 mmol/L in, e.g., Ethanol)*

~10 min heating (molecule binding & solvent removal)

Rinsing with ethanol (Removal of unbound molecules)

Method 2: Spin coating

suitable for fast research and optimization

Spin-coating‡ of SAM forming agent solution at min. concentration of 0.5 mmol/L

~10 min heating (rinsing is optional)

* The minimum needed dipping time can vary from minutes to hours. After some further testing with 2PACz, researchers found more reproducible results with rather 0.5 mmol/L and 5 min dipping. Note that optimal concentration and dipping time may vary depending on the used substrate oxide and pre-treatment.

- **The SAM forming agents can be processed within wide processing windows with higher reproducibility than current standard hole transport materials (like PTAA). The substrates (e.g. ITO) have to be clean and activated by, for example, UV-Ozone treatment.**

- **The SAM forming agent powders were usually dissolved in ethanol or isopropanol (1 mmol/L ≈ 0.3 mg/mL), MeO-2PACz powder was stored in air, while 2PACz and Me-4PACz were stored in a nitrogen gas-filled glovebox. MeO-2PACz can be exposed to air when in use [and is not air-sensitive], however, because of its long storage time and useful life, TCI recommends storing the product under inert gas to ensure maximum efficacy over time.**

‡For more details, see supplementary information of the following reference.

A. Al-Ashouri, A. Magomedov, V. Getautis, S. Albrecht, *et al*., *Energy Environ. Sci*. **2019**, *12*, 3356. https://doi.org/10.1039/C9EE02268F

*These data are provided by Prof. Steve Albrecht and Prof. Vytautas Getautis.

For further information please refer to our website at www.TCIchemicals.com. ▶▶▶ TCI solar cell

Ordering and Customer Service

TCI AMERICA
Tel : 800-423-8616 / 503-283-1681
Fax : 888-520-1075 / 503-283-1987
E-mail : Sales-US@TCIchemicals.com

TCI EUROPE N.V.
Tel : +32 (0)3 735 07 00
Fax : +32 (0)3 735 07 01
E-mail : Sales-EU@TCIchemicals.com

TCI Deutschland GmbH
Tel : +49 (0)6196 64053-00
Fax : +49 (0)6196 64053-01
E-mail : Sales-DE@TCIchemicals.com

Tokyo Chemical Industry UK Ltd.
Tel : +44 (0)1865 78 45 60
E-mail : Sales-UK@TCIchemicals.com

梯希爱(上海)化成工业发展有限公司
Tel : 800-988-0390 / 021-67121386
Fax : 021-6712-1385
E-mail : Sales-CN@TCIchemicals.com

Tokyo Chemical Industry (India) Pvt. Ltd.
Tel : 1800 425 7889 / 044-2262 0909
E-mail : Sales-IN@TCIchemicals.com

TOKYO CHEMICAL INDUSTRY CO., LTD.
Tel : +81 (0)3-5640-8878
E-mail : globalbusiness@TCIchemicals.com