Functionality-Directed Screening of Pb-Free Hybrid Organic–Inorganic Perovskites with Desired Intrinsic Photovoltaic Functionalities

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$[CH_3NH_3]P\ I_3$ (1.5 V)[27,28] a $[CH_3NH_3]P\ B_3$ (2.35 V)[29]
          i a a   1.34 V   S   −Q   i
i i,[30]   a i i   a   i   a i
    a i   i   i   a   a   i i
    a a ,   i   a ia a a   i i a a   a
      i i   −   a   ,[31]   .

Can the Current Limitations Be Overcome by Identifying Other Compounds from the Same General Group? I   i   a i   a   a i $AM^{IV}X^{VII}_3$ a   ia
          a   i   i   a   i i a i   .
Gi   a   i   i   a   (
Fi   1a)   a   i   A = $CH_3NH_3^+$,

$CH(NH_2)_2^+$, $M^{IV} = P$ a $X^{VII} = I, B$,[10,11,13,22,24,32−36]
a   i   i   a   a   a   a   a
                                                          . A
      a   a i   a   ia   a   i   a   i
a   i   i   a   i   a i i
        i   i .[37−39] I   i a   ,   a ia   i
  ia   a i a i   a i   i   a a   a   i
      i   ia -a -   i   a   a   a
      a i . T   a   ia   i   -
      i a ,   a   i   a   i
      a a   i i a,   a ia -   i "   " (DP)
    a   a   ia   i i   a -   i   .
T   i   a   "
   $t_{,,,}$" (DM),   i   i   DP ,   i
      i   a i   a   a a   a i i . I
    a a   a   i PV a ia ,   i   a
          a   i   a i   i   i
DM ,   ia   - i i   i
      .[40,41] I   i i ,   DM a   i i   i i i
      a ia   i   a   PV   a   a
i   a   i ,   a , a i   i i ,   i a-
i   i i i ,   a   a i   ,   .   i   a   i -

i   ia a   i   i   i   (a i
Si a   PV   a   ). H   ,   a i a i
              i   i   a i −i   a i   i
a i   a   i   i a   a   i   a i
a   a .[42−45]
    H   a   a   i   a i - i   a   ia   i
a   a   ia   i   - i i   a   a i
      ia i -   a   PV   i $AM^{IV}X^{VII}_3$ i .
S   a   a i i a,   i - a   a   a   a
              a   i   i   i a
i   i a i a   a   a   a i a i   i
18-   Ha -H   i   a   .[46,47] W   i
      i i i /   a   a   i
    i   a   a i   a   . T   a a
              i   a   ia   i   a   i
      i   ia i   i i   (a
      i   a i a   i a i) a   (4449(( )-
XVII
  3

i   i   ′′ ′ *t* ′ *t* . O   ai   i a   a   a
                     a   i - a   i i   i a a
(i. .,   i   i i   i S   i   2)   a
        a   ai   i   i

i a   a   a   i   P X^{VI}.[53] T   i i   a
X^{VII}–   a   M^{IV}–   i i a i   i VB   a   a i a
a   ia i a a   i Fi   5. T
DM   * a   * a   i Fi   7. I
i   a   i   i   a   a
a - a i   i i   i . O
i   i ,   , a a   ii   i
a   i   a i   i , i , i
a   a   i   , i   i
F   i i   a i . T   i   a   a
i -   a   i i   i ,   i
a   i   a ia   i a   ii .

(4) Su ciently Low Binding Energy and Large Localization Radius for Electron–Hole Pairs. O
a   a   i   a   a   i
a   —   ai (i . ,   i   )
a   i   a a   i   i   i a-
i . T i i   a a   i   i

4+.[84,85] (iii) A ... a ... i ... a ... i ... N ... a G-a ...[79,80] iii ... [FA]PbI$_3$, ...[86]

W ... *t* ... (Fig 3) ...

... AM^{IV}X$^{VII}_3$ ... $0.81 < t < 1.11$ and $0.44 < ... < 0.90$.[87] W ... *t*, ... [EA, GA, DEA]GeCl$_3$ ... 1.11. T ... . T ... Fig 3 ... AM^{IV}X$^{VII}_3$ ... *t*. G ... : Pm$\bar{3}$m/S ... *t* < 0.97 (...) a ... G ... *t* > 0.97 (...). F ... *t*, ... (i. ., ...). T ... [88] ... *t* 1.0 ... AM^{IV}X$^{VII}_3$ ... . A ... *t* (<0.89), ... [CH$_3$NH$_3$]PbI$_3$, ... M^{IV}X$^{VII}_6$ ...) ... .[49] I ... / ... . T ... AM^{IV}X$^{VII}_3$ ...

.[28,38,49] T ... i P-a ... S-a ... G-a ...

a   *a   a   a   *,   i   i i i
               a   i   i   i   *
a i   *. B   * a   *   i   a i
i i   i   i . F   S   a   G   a
          ,   a   a   * i   a i   i   i
A⁺   a i   . T   a   ʃ (Fi   6),
i   a   i   a   i /

$M^{IV}-X^{VII}$