

Composition and impurity analysis of light absorbers of perovskite-based solar cells

It is important to figure out the concentration of composition and impurity of light absorbers to achieve high efficiency in perovskite-based solar cells. For the analysis of inorganic elements, ICP-AES, ICP-MS and ion chromatography are available.

Menu of elemental analyses of light absorbers

H																					He
Li	Be									B	C	N	O	F							Ne
Na	Mg									Al	Si	P	S	Cl							Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br					Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I					Xe
Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At					Rn
Fr	Ra	A																			
		L	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu				
		A	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr				

E Inductively coupled plasma-mass spectrometry (ICP-MS)
E Inductively coupled plasma-atomic emission spectrometry (ICP-AES)
E Ion chromatography (IC)
E Other methods may be available.

Since ICP-MS, ICP-AES and IC accept solution in analyses, samples must be brought into solution before measurements.

- ICP-MS : analyze produced ion via mass spectrometer after introducing the sample solution into plasma. High sensitivity
- ICP-AES : analyze emission radiated from atoms and/or ions after introducing the sample solution into plasma. High repeatability
- IC : analyze ionic species in sequence passing through a separation column, where ions separate based on chemical properties.

Practical elemental analyses of light absorbers

Trace metal analysis via ICP-MS

(Unit : $\mu\text{g/g}$)

	MAPbI ₃ ·DMF	FAPbI ₃ ·2DMF
Li	<0.5	<0.5
Na	1	5
P	<2	<2
K	0.9	<0.5
Ti	<0.5	<0.5
Fe	<0.5	<0.5
Ge	<0.5	<0.5
Rb	<0.5	<0.5
Rh	<0.5	<0.5
Sn	<0.5	<0.5
Cs	<0.5	<0.5

- Approximately 60 kinds of metal elements can be evaluated at ppm level.
- High resolution ICP-MS enables sensitive quantification of P and Rh, which are difficult to be evaluated using conventional quadrupole mass spectrometer.

Composition analysis via ICP-AES

(Unit : mass%)

	MAPbI ₃ ·DMF	FAPbI ₃ ·2DMF
Pb	29.7	32.2
I	56.8	61.5
I / Pb	3.13	3.12

Note) The 3rd digit is indicated of reference.

- Possible to obtain the compositional ratio of Pb and I.
- Necessary to avoid loss of Pb and I at sample preparation.

Analysis of halogen via IC

(Unit : mass%)

	MAPbI ₃ ·DMF	FAPbI ₃ ·2DMF
F	<1	<1
Cl	<10	<10
Br	<3	<3

- Possible to analyze halogens, including I, at mass% level. Halogens extracted from samples by pure water can be evaluated at ppm level.

Metal impurities in light absorbers can be evaluated with high sensitivity via ICP-MS. Composition analysis can be accomplished via ICP-AES, note, however, that appropriate sample preparation is required.

Samples are provided by Prof. Atsushi Wakamiya, Kyoto University.