Welcome to

Confirmed Invited Speakers (alphabetical order):

Ryu Abe, Japan
Detlef Bahnemann, Germany
Christophe Colbeau-Justin, France
Michael R. Hoffmann, USA
Marcin Janczarek, Poland
Agata Markowska-Szczupak, Poland
Teruhisa Ohno, Japan
Bunsho Ohtani, Japan
Jeremy Pietron, USA
Michael Wark, Germany
Adriana Zaleska-Medynska, Poland
…

www.cat.hokudai.ac.jp/icat-nepec

Frontiers in Chemistry (IF = 3.994)

A **high visibility** journal publishing **outstanding, interdisciplinary** research across **the chemical sciences.**

frontiers

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2200+ Editors

Field Chief Editor

Steve Suib (The University of Connecticut Storrs, USA)

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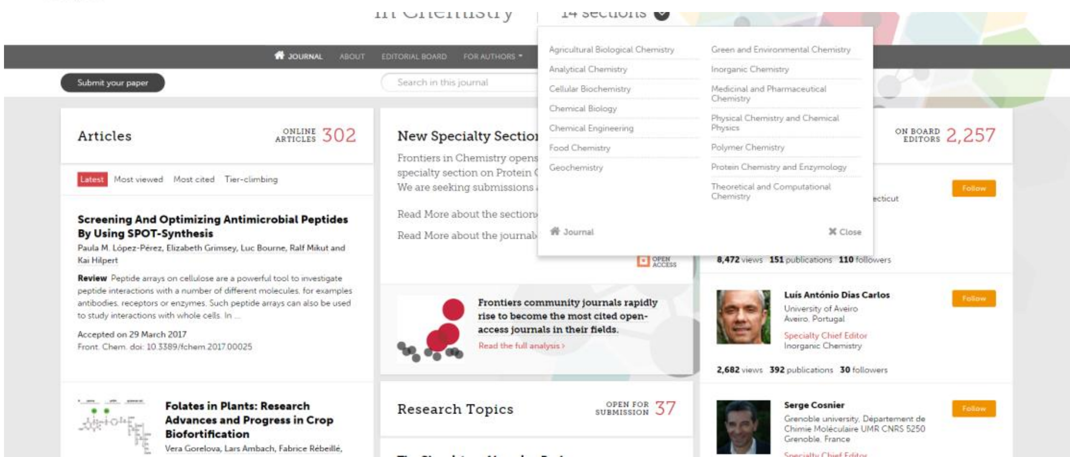
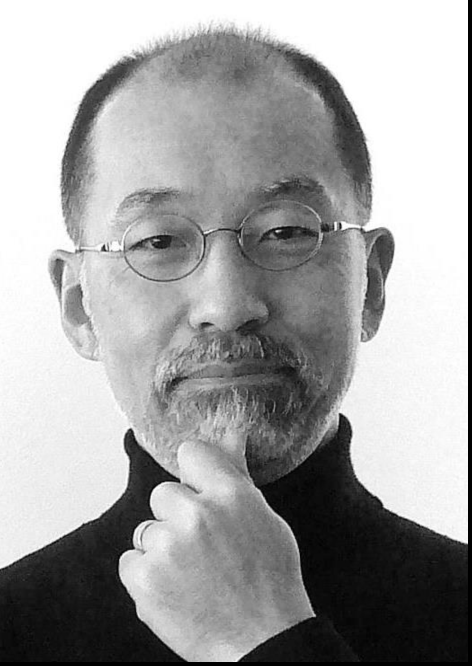
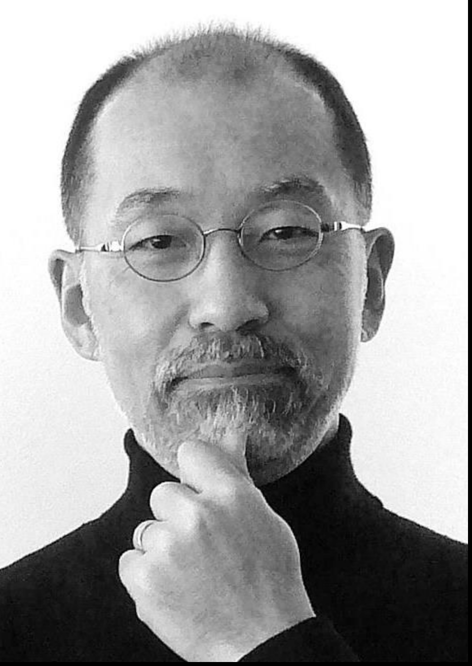




Bunsho OHTANI
大谷文章



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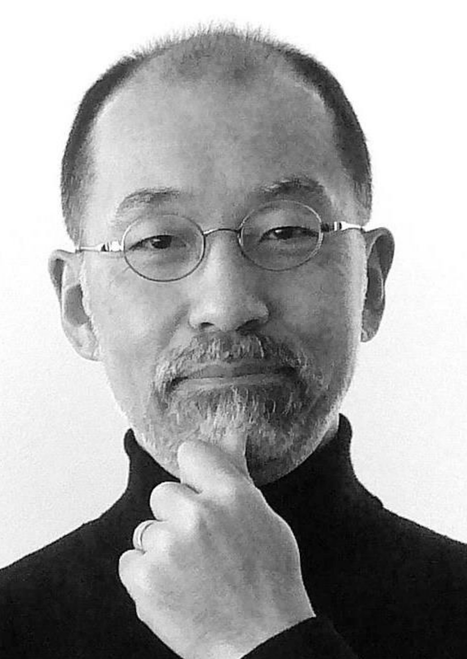
大谷文章

ohtani@cat.hokudai.ac.jp



Bunsho OHTANI
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unique

ユニーク

ICAT

Institute for Catalysis, Hokkaido University

Sapporo 001-0021, Japan

founded originally in 1943

Hokkaido University

- one of the former 8 imperial universities
- founded as Sapporo Agricultural College in 1876

William S. Clerk

The first principal of Sapporo Agricultural College, the former of Hokkaido University

clerk@sapporo-agri.ac.jp

William S. Clerk

The first principal of Sapporo Agricultural College, the former of Hokkaido University

clerk@sapporo-agri.ac.jp

Boys be ambitious!
(BBA)

ambitious

ambi-	environmental/both sides
ambient	completely enveloping/surrounding
ambivalent	uncertain or unable to decide about what course to follow
ambidextrous	equally skillful with each hand
ambitious	having a strong desire for success or achievement

ambitious

ambiguous = not clear

はっきりしない（あいまい）

ambiguous = not clear

はっきりしない（あいまい）

unambiguous = not not-clear

ambiguous ＝ not clear

はっきりしない（あいまい）

unambiguous ＝ not not-clear

「はっきりしない（あいまい）」じゃない

ambiguous ＝ not clear

はっきりしない（あいまい）

unambiguous ＝ not not-clear

「はっきりしない（あいまい）」じゃない

≠ clear・はっきり

science/科学

science/科学

unambiguousness + text

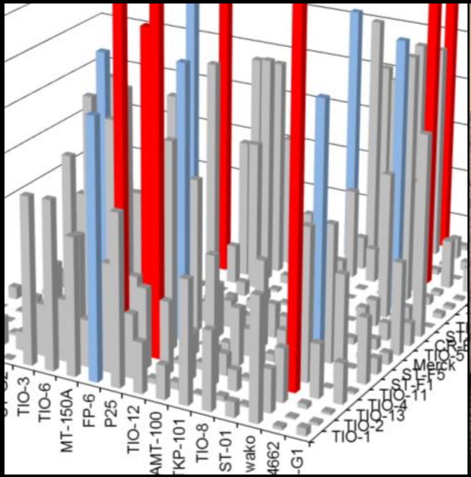
あいまいじゃない＋ことばであらわす

A Novel Concept of Identification of Metal-oxide Powders by Energy-resolved Density of Electron Traps

identification

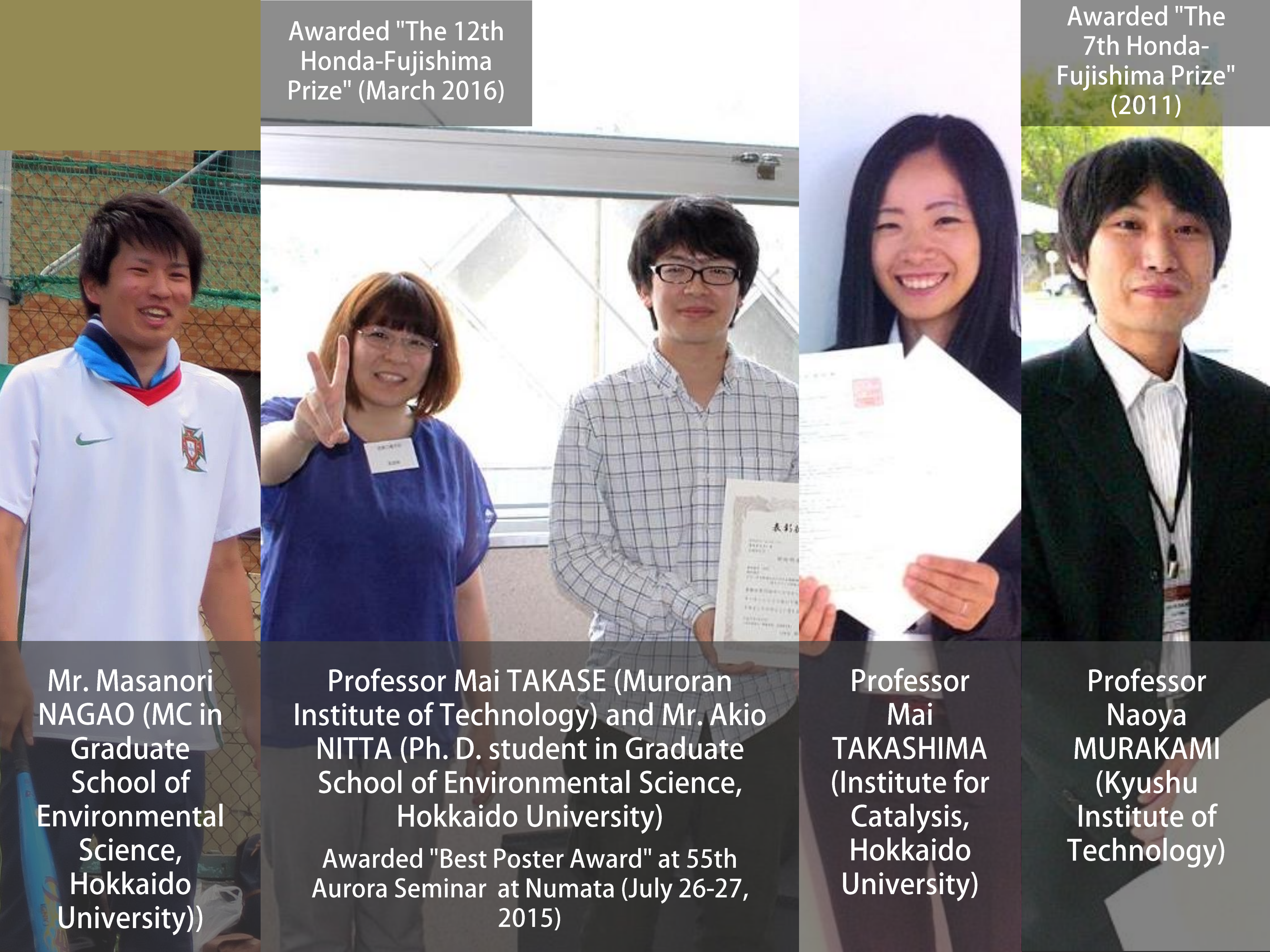
fingerprint

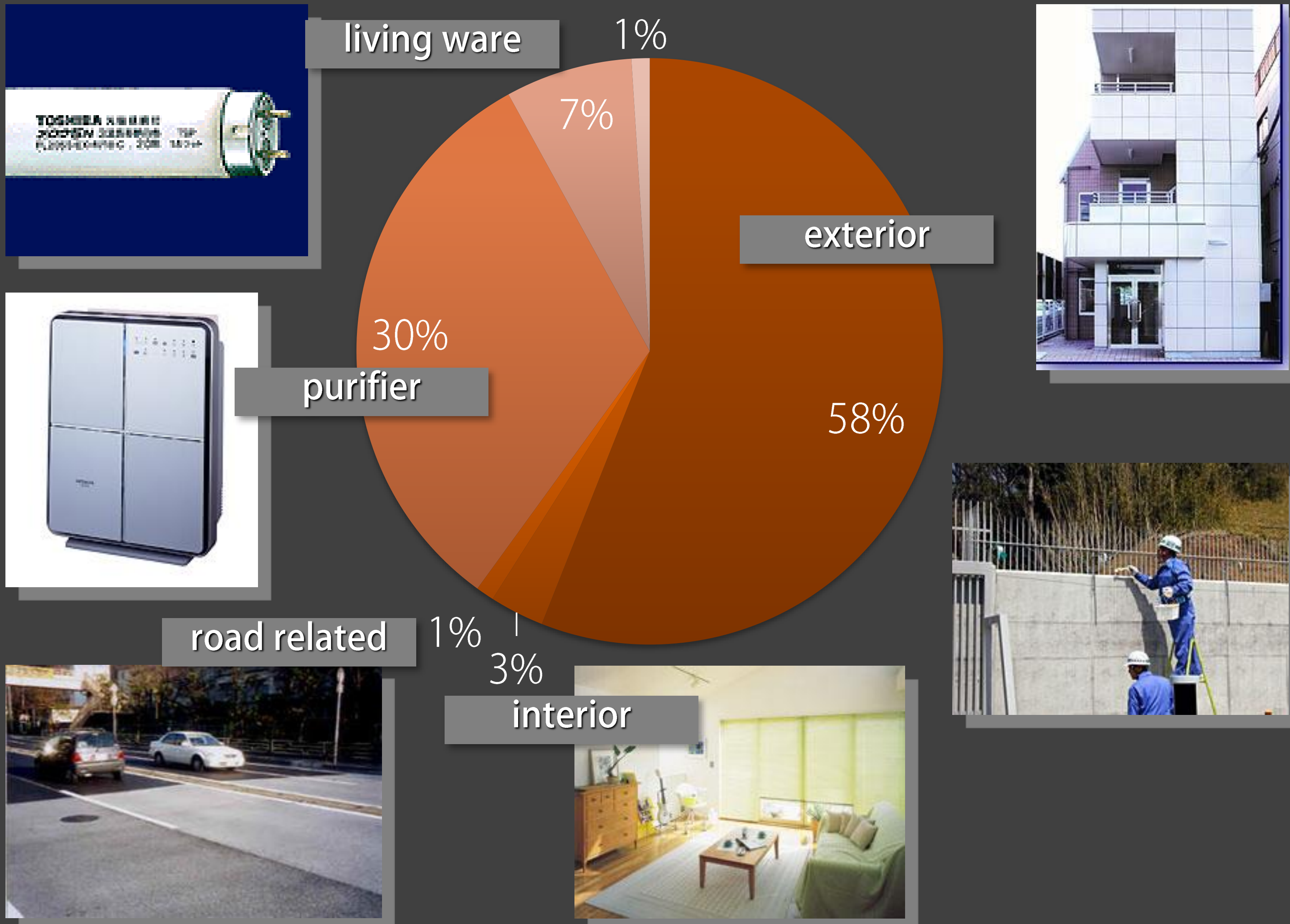
coincidence



correlation

Bunsho OHTANI (Hokkaido University, Japan)


Awarded "The 12th Honda-Fujishima Prize" (March 2016)
Awarded "The 7th Honda-Fujishima Prize" (2011)
Mr. Masanori NAGAO (MC in Graduate School of Environmental Science, Hokkaido University))
Professor Mai TAKASE (Muroran Institute of Technology) and Mr. Akio NITTA (Ph. D. student in Graduate School of Environmental Science, Hokkaido University)
Awarded "Best Poster Award" at 55th Aurora Seminar at Numata (July 26-27, 2015)
Professor Mai TAKASHIMA (Institute for Catalysis, Hokkaido University)
Professor Naoya MURAKAMI (Kyushu Institute of Technology)



photocatalysis industries in Japan = ca. 350 million USD (2015)

Fujishima, A.; Honda, K., *Nature* **238**, 37 (1972).

Electrochemical Photolysis of Water at a Semiconductor Electrode

Although the possibility of water photolysis has been investigated by many workers, a useful method has only now been developed. Because water is transparent to visible light it cannot be decomposed directly, but only by radiation with wavelengths shorter than 190 nm (ref. 1).

For electrochemical decomposition of water, a potential difference of more than 1.23 V is necessary between one electrode, at which the anodic processes occur, and the other, where cathodic reactions take place. This potential difference is equivalent to the energy of radiation with a wavelength of approximately 1,000 nm. Therefore, if the energy of light is used effectively in an electrochemical system, it should be possible to decompose water with visible light. Here we describe a novel type of photo-electrochemical cell which decomposes water in this way.

Electrolysis of water can occur even without applying electric power if one of the following three conditions is fulfilled. First, oxygen evolution occurs at a potential more negative than that at which hydrogen evolution occurs in normal conditions; second, hydrogen evolution occurs at a potential more positive than that at which oxygen evolution occurs in normal conditions; third, the potential for oxygen evolution is made more negative and that for hydrogen evolution is made more positive, until the former is more negative than the latter.

Current–voltage curves of a semiconducting n-type TiO_2 electrode have been measured with a static potentiometer in the dark and under irradiation with light[2] (Fig. 1). Anodic current which is proportional to the intensity of light begins to flow for wavelengths shorter than 415 nm, that is 3.0 eV, which corresponds to the band gap of TiO_2. The current reaches saturation at potentials positive relative to a saturated calomel electrode (SCE). These facts suggest that the anodic reaction is related to the formation of holes in the valence band by light excitation. Oxygen evolution was confirmed by several means of analytical measurements[3,4]. Oxygen evolution occurs at −0.5 V (SCE) in an aqueous electrolyte of *p*H 4.7; this is more negative than the standard potential. We have termed such behaviour "photosensitized electrolytic oxidation" (ref. 2). When halogen ions were introduced in the electrolyte, they were also oxidized through the suggested mechanism of photosensitized electrolytic oxidation. This also occurred with other types of n-type semiconductor such as ZnO and CdS (ref. 5). We believe therefore that the oxygen evolution reaction on the TiO_2 electrode under irradiation belongs to the first category described above.

We then constructed an electrochemical cell in which a TiO_2 electrode was connected with a platinum black electrode through an external load (Fig. 2). When the surface of the TiO_2 electrode was irradiated, current flowed from the platinum electrode to the TiO_2 electrode through the external circuit. The direction of the current reveals that the oxidation reaction (oxygen evolution) occurs at the TiO_2 electrode and reduction (hydrogen evolution) at the platinum black electrode.

We suggest that water can be decomposed by visible light into oxygen and hydrogen, without the application of any external voltage, according to the following schemes:

$$TiO_2 + 2\,h\nu \rightarrow 2\,e^- + 2\,p^+ \qquad (1)$$
(excitation of TiO_2 by light)

$$2\,p^+ + H_2O \rightarrow \tfrac{1}{2}\,O_2 + 2\,H^+ \qquad (2)$$
(at the TiO_2 electrode)

$$2\,e^- + 2\,H^+ \rightarrow H_2 \qquad (3)$$
(at the platinum electrode)

The overall reaction is

$$H_2O + 2\,h\nu \rightarrow \tfrac{1}{2}\,O_2 + H_2 \qquad (4)$$

The starting potential of the oxidation reaction at the TiO_2 electrode corresponds almost exactly to the flatband potential which is constant in the electrolyte solution of a given *p*H. To increase the efficiency of the decomposition process, more reducible species, for example, dissolved oxygen or Fe^{3+} ions, must be added in the compartment of the platinum electrode. When Fe^{3+} ions were added, the current produced under irradiation increased. Currents of a few mA flowed when the TiO_2 electrode (surface area ~1 cm^2) was irradiated by a 500 W xenon lamp; we estimate the quantum efficiency in this case to be approximately 0.1. The e.m.f. of the cell was measured to be up to 0.5 V.

It is possible that the hydrogen evolution reaction shifts towards more positive potential than normal when suitable p-type semiconductor electrodes are irradiated, in the same way that photosensitized oxygen evolution occurs with n-type semiconductor electrodes. If such a p-type semiconductor electrode is used instead of the platinum electrode, electrochemical photolysis of water may occur more effectively.

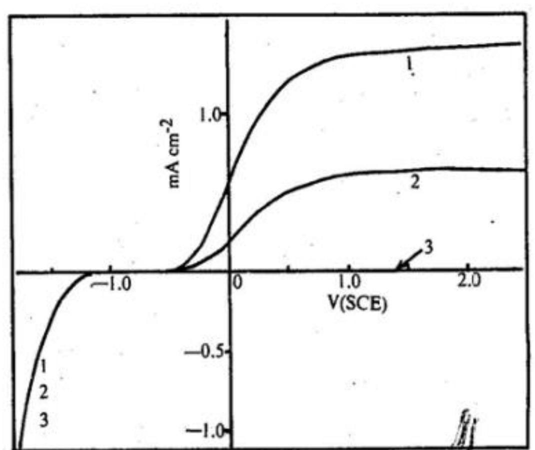


Fig. 1 Current–voltage curves for TiO_2 n-type semiconductor. A single crystal wafer of n-type TiO_2 (rutile) was used after treatment at 700° C at $10^{-4} \sim 10^{-5}$ torr for roughly 4 h to increase the conductivity of the crystal. This wafer was approximately 1.5 mm thick and the exposed (001) surface area was approximately 1.0 cm^2. Indium was evaporated on to one side of the surface to ensure ohmic contact and a copper lead wire was connected on the indium layer with silver paste. All other surfaces were sealed by epoxy resin.

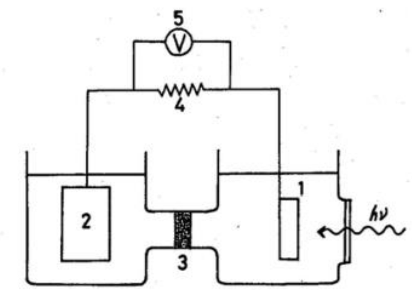


Fig. 2 Electrochemical cell in which the TiO_2 electrode is connected with a platinum electrode (see text). The surface area of the platinum black electrode used was approximately 30 cm^2.

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Received September 13, 1971; final revision April 24, 1972.

1 Coehn, A., *Ber. Deutsch. Chem. Gesellschaft*, **43**, 880 (1910).
2 Fujishima, A., Honda, K., and Kikuchi, S., *J. Chem. Soc. Japan (Kogyo Kagaku Zasshi)*, **72**, 108 (1969).
3 Fujishima, A., and Honda, K., *J. Chem. Soc. Japan*, **74**, 355 (1971).
4 Fujishima, A., and Honda, K., *J. Institute of Industrial Science, University of Tokyo (Seisan Kenkyu)*, **22**, 478 (1970).
5 Fujishima, A., Sugiyama, E., and Honda, K., *Bull. Chem. Soc. Japan*, **44**, 304 (1971).

Electrochemistry

The Electrochemical Society of Japan

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JOI:DN/JST.JSTAGE/electrochemistry/82.414

Review *Electrochemistry*, **82(6)**, 414–425 (2014)

Revisiting the Original Works Related to Titania Photocatalysis: A Review of Papers in the Early Stage of Photocatalysis Studies

Bunsho OHTANI*

Catalysis Research Center, Hokkaido University, Sapporo 001-0021, Japan

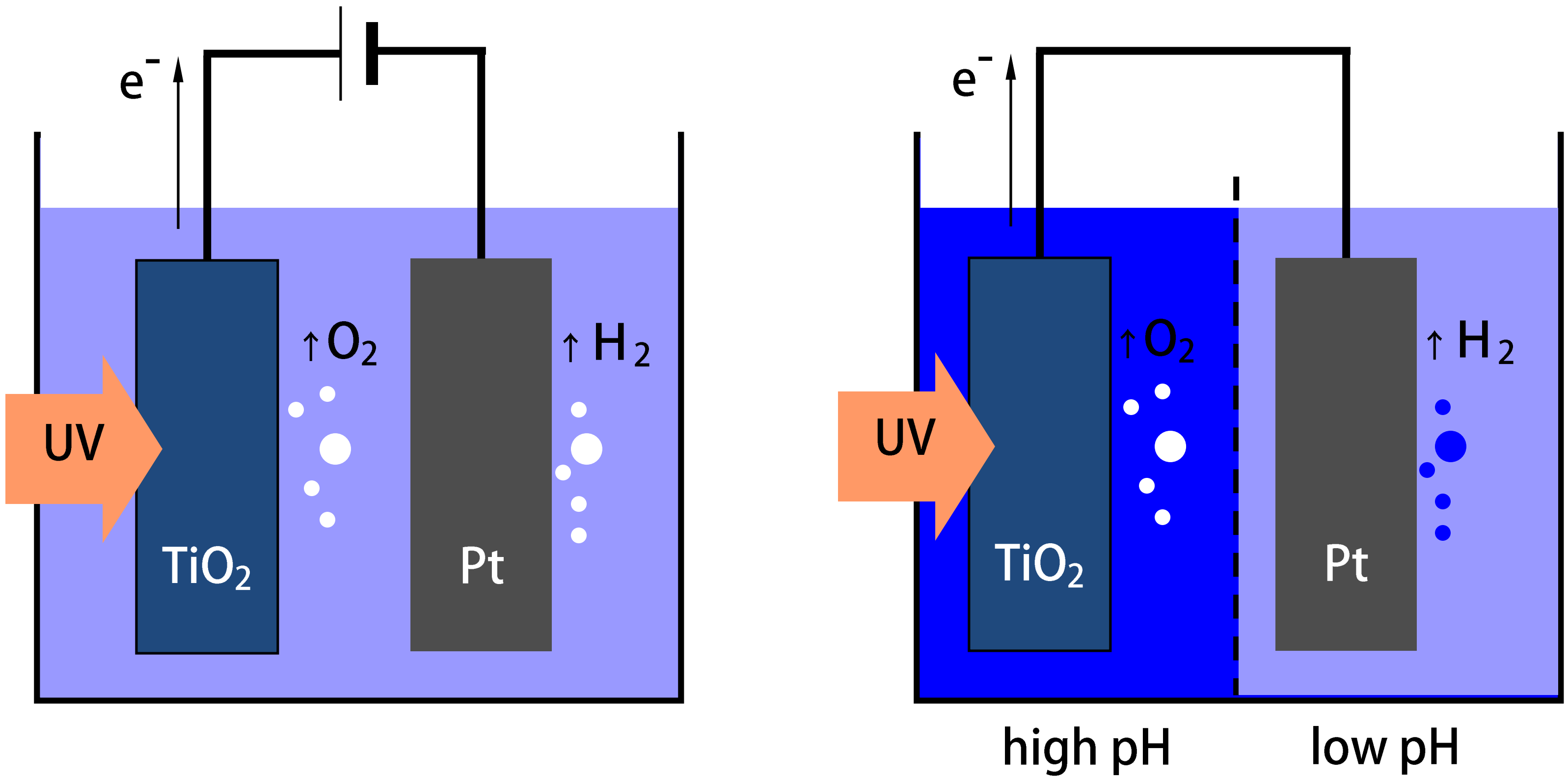
Checked by several electrochemists:

63) A. Nozik, *Nature*, **257**, 383 (1975).
64) M. S. Wrighton, D. S. Ginley, P. T. Wolczanski, A. B. Ellis, D. L. Morse, and A. Linz, *Proc. Natl. Acad. Sci. U.S.A.*, **72**, 1518 (1975).

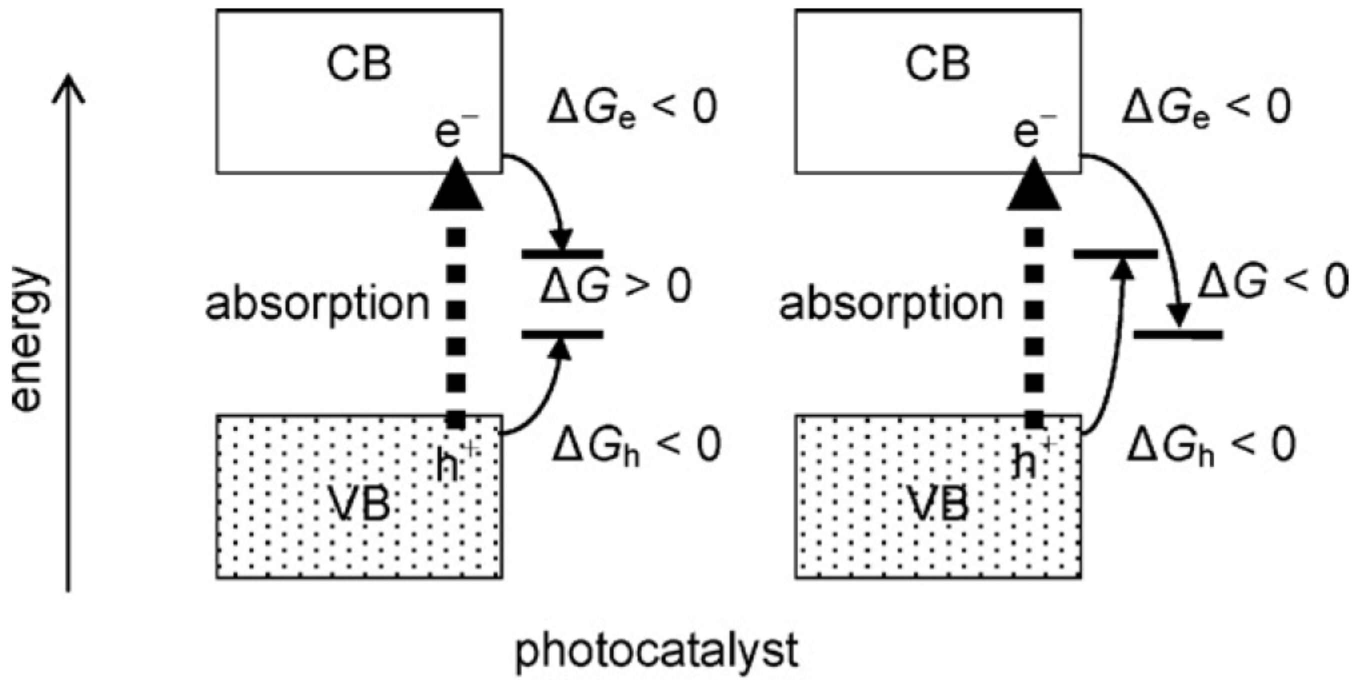
H: Honda-Fujishima effect

hidden message

requirement of BIAS potential, i.e., electric FIELD in the BULK to separate photoexcited electron and positive hole (= charge separation) to drive the reactions of positive Gibbs energy change



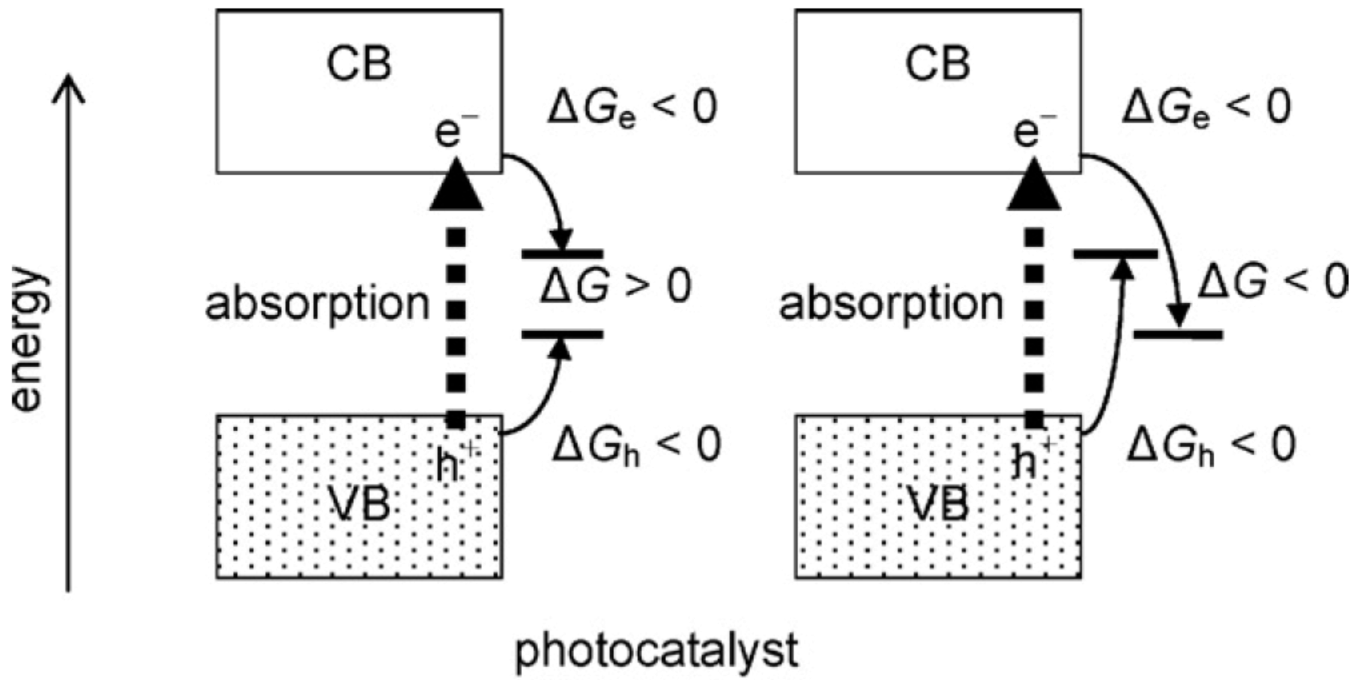
J. Photochem. Photobiol. C: Photochem. Rev., **11**, 157 (2010)



(1) thermodynamics = no kinetics

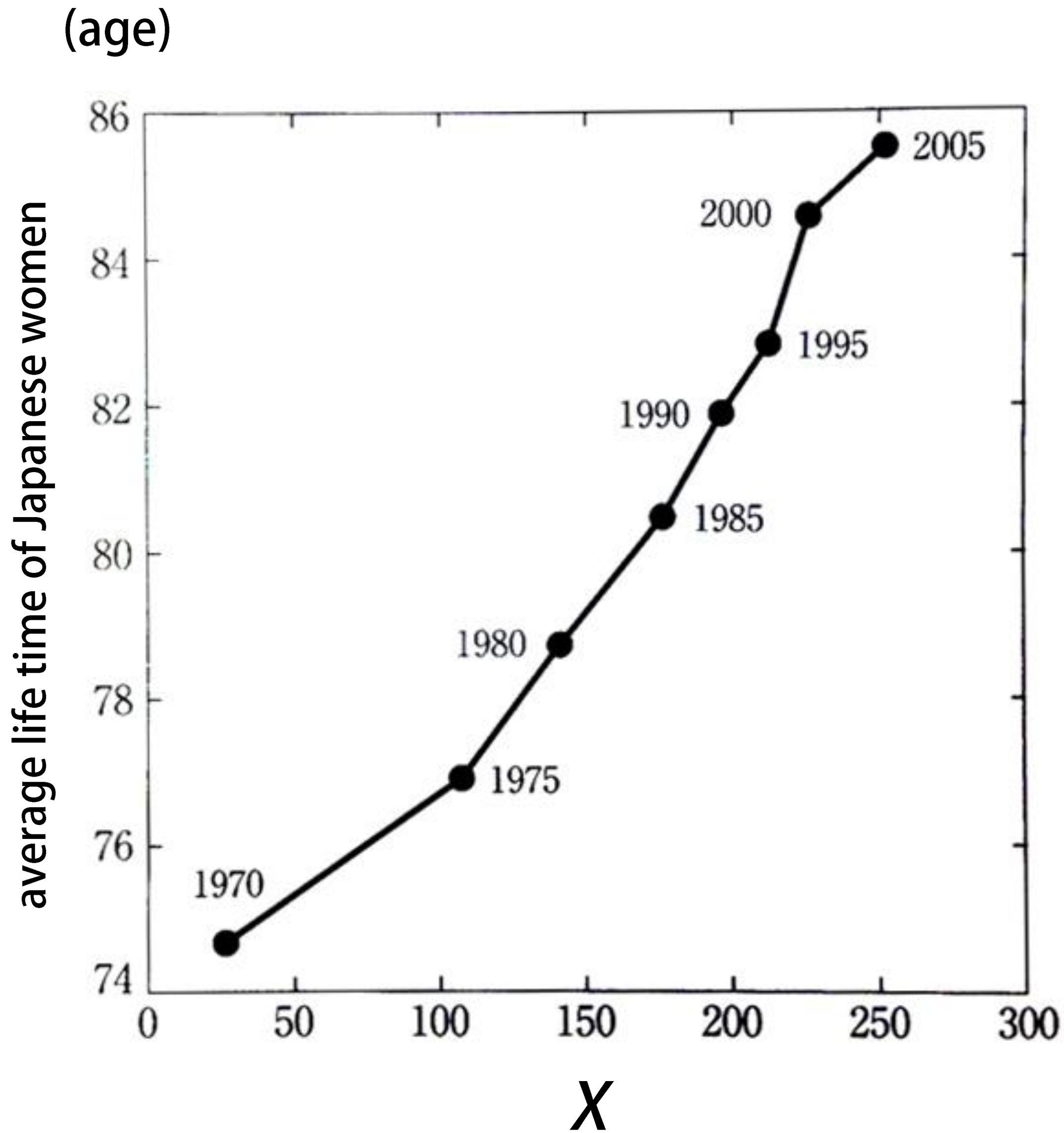
(2) single electron transfer only

J. Photochem. Photobiol. C: Photochem. Rev., **11**, 157 (2010)

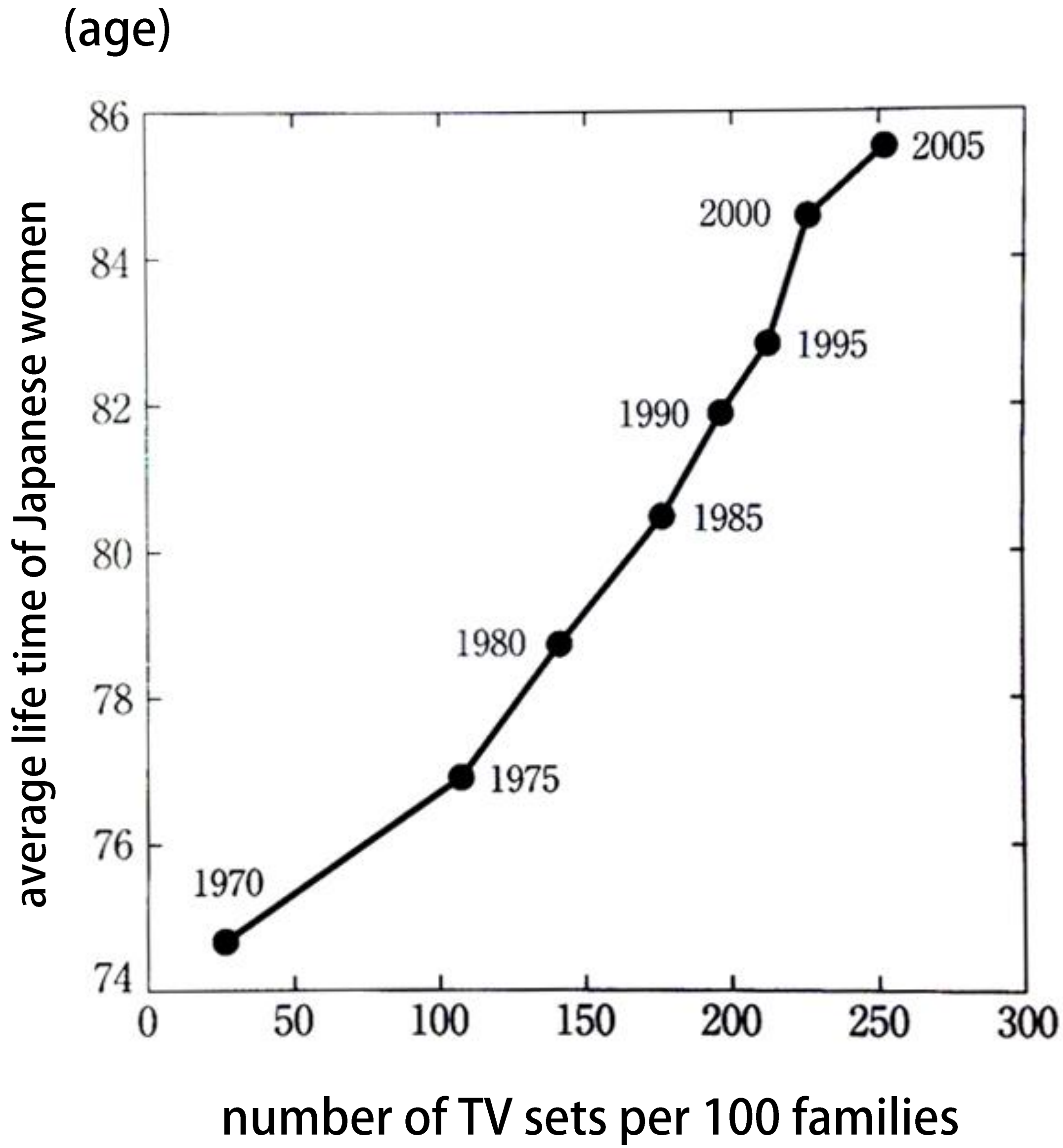


no IDENTIFICATION of photocatalyst powders

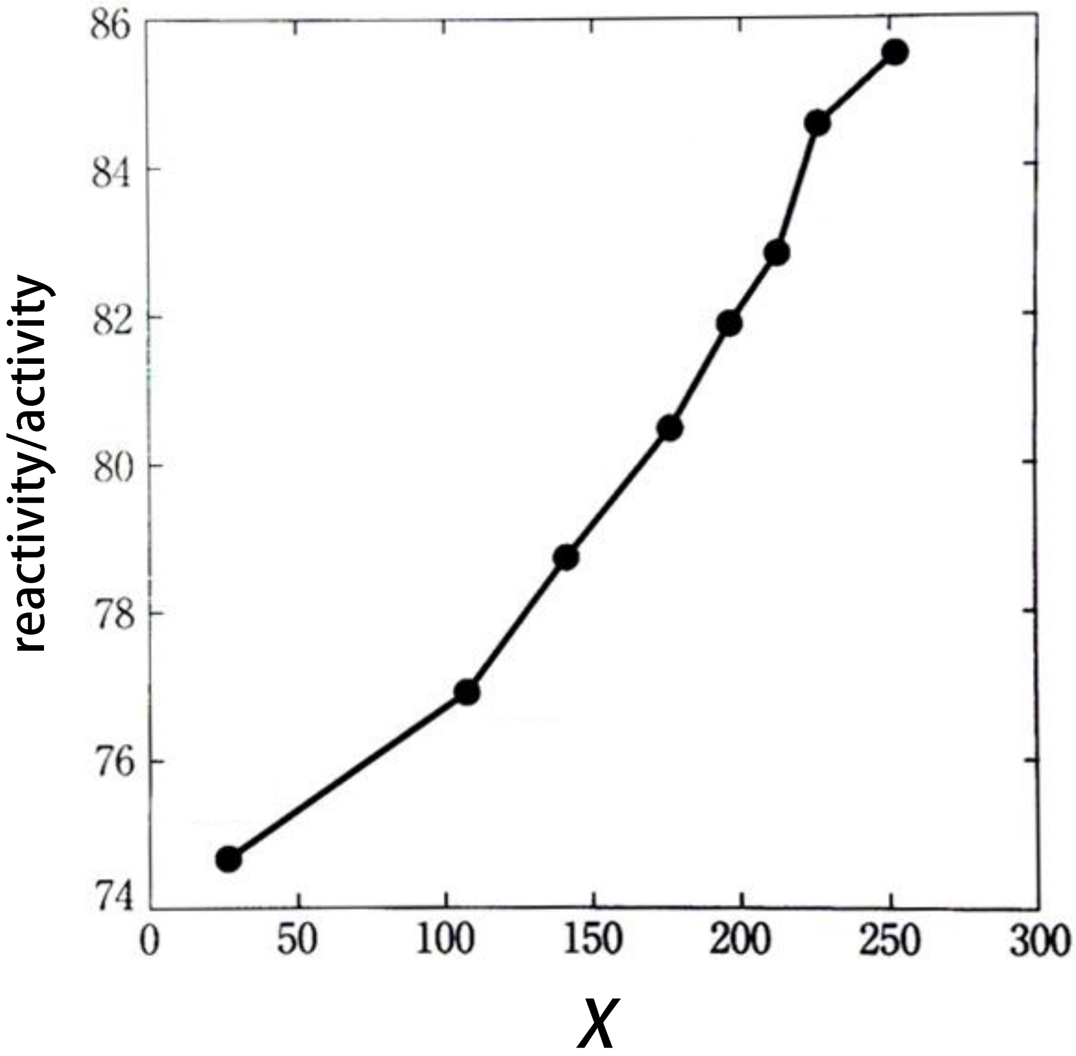
J. Photochem. Photobiol. C: Photochem. Rev., **11**, 157 (2010)



「もうダマされないための『科学』講義」菊池誠・松永和紀・伊勢田哲治・平川秀幸・片瀬久美子・飯田泰・SYNODOS，光文社新書（2011）



「もうダマされないための『科学』講義」菊池誠・松永和紀・伊勢田哲治・平川秀幸・片瀬久美子・飯田泰・SYNODOS，光文社新書（2011）



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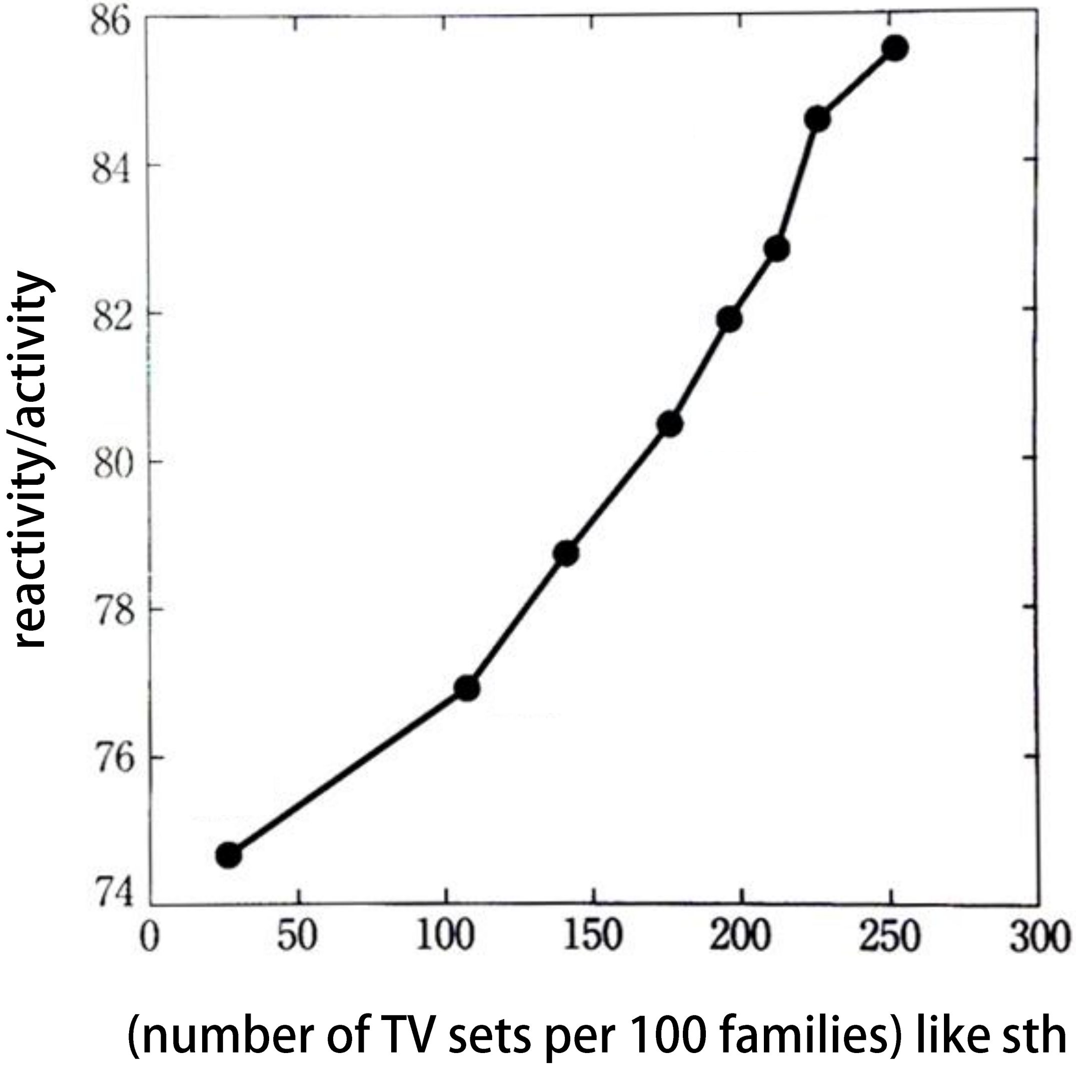


「もうダマされないための『科学』講義」菊池誠・松永和紀・伊勢田哲治・平川秀幸・片瀬久美子・飯田泰・SYNODOS，光文社新書（2011）

X

e.g., titania particles

composition: TiO_2

crystalline form: anatase/rutile ...

particle size

specific surface area

?

identification

物質の同定

benzene


021-00716
Wako
Benzene
ベンゼン
500ml
AWN0625
Triple Benzenes
Yoneyama Extra Pure Reagent
Benzene
ベンゼン
Requirements
米山薬品工業株式会社
SHOWA
昭和一級
ベンゼン
Benzene

structure (purity)

構造（純度）

science/科学

unambiguousness + text

あいまいじゃない + ことばであらわす

identification of organic compounds

e.g., *J. Org. Chem.* (ACS) requests identification by at least:

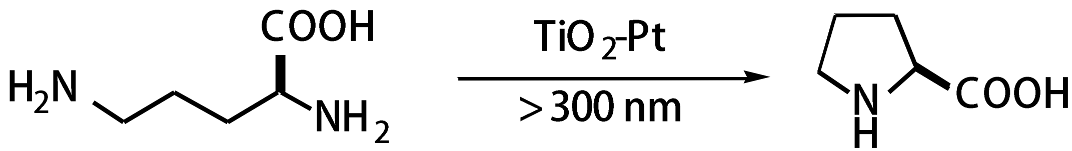
✓ elemental analysis data within 0.3% error
composition and purity

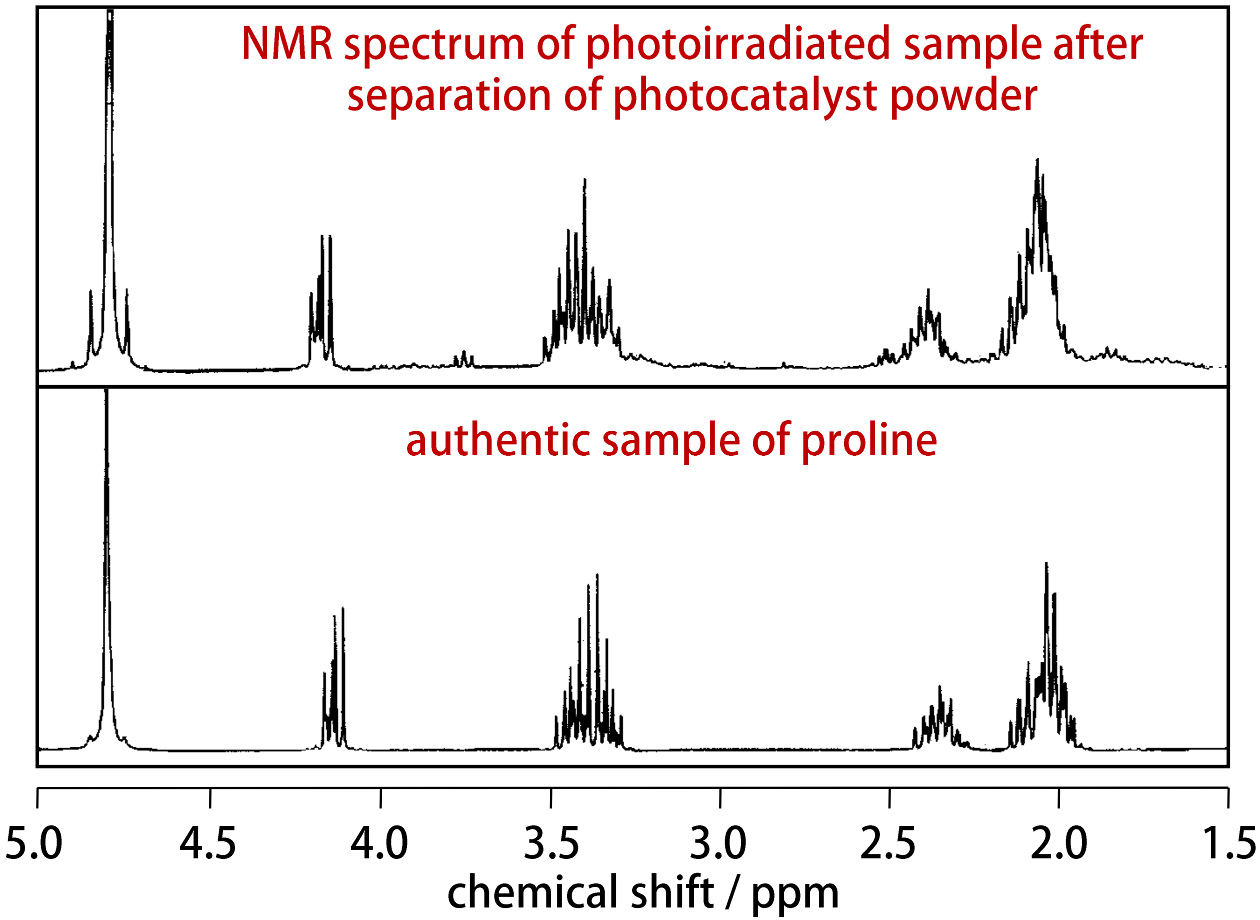
✓ nuclear magnetic resonance pattern
skeleton

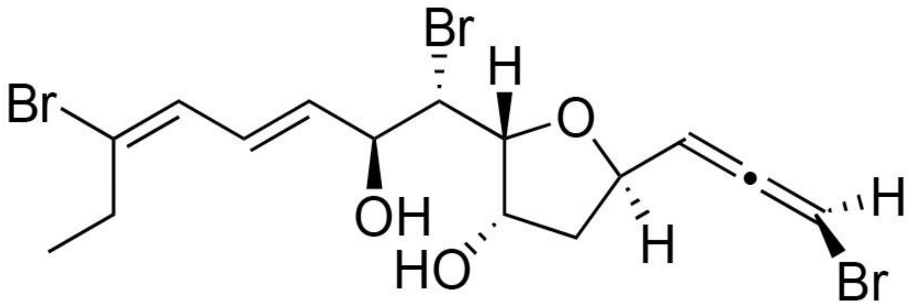
Wienbibliothek, Tagblattarchiv, photos collection, TF-008286

identification of organic compounds

Ohtani, B.; Tsuru, S.; Nishimoto, S.-i.; Kagiya, T.; Izawa, K. *J. Org. Chem.* **1990**, *55*, 5551-5553. [64]

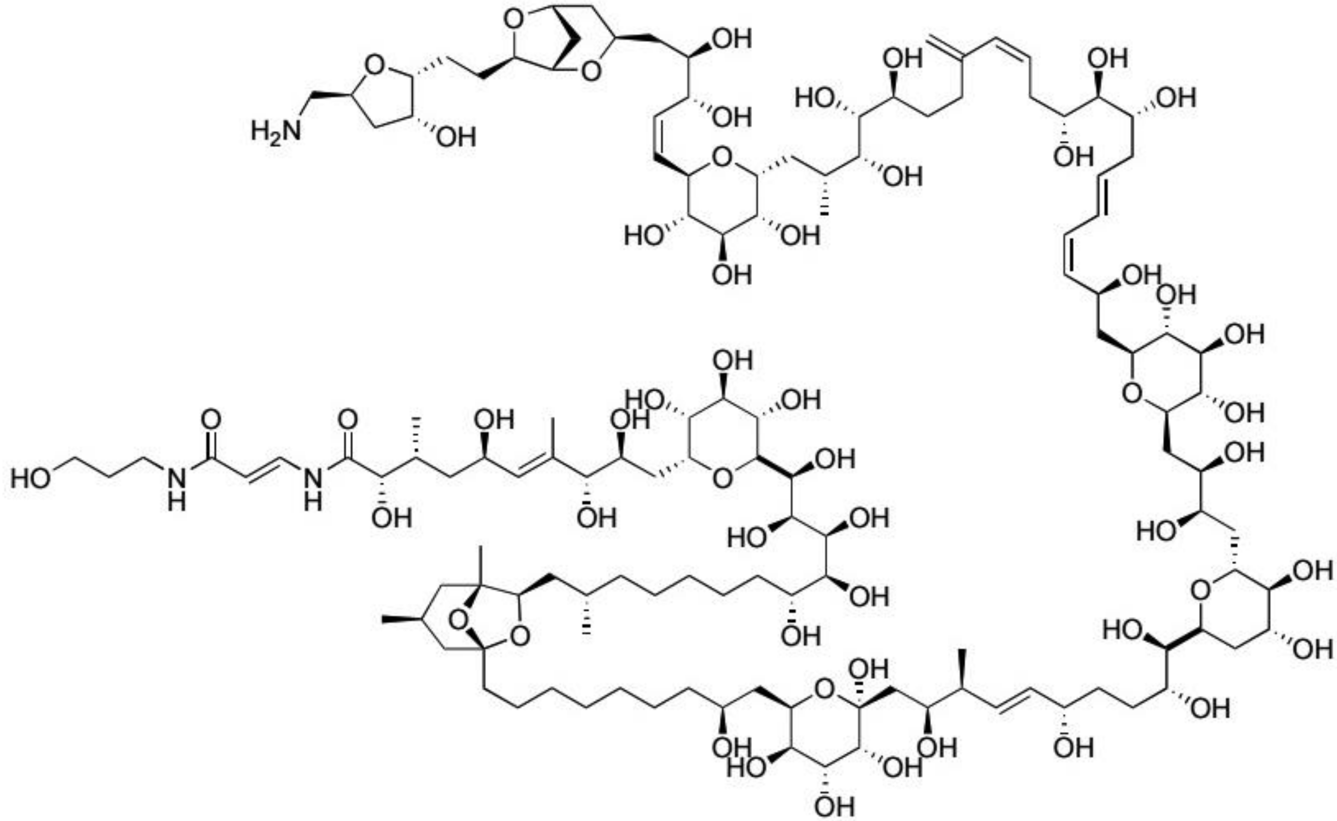




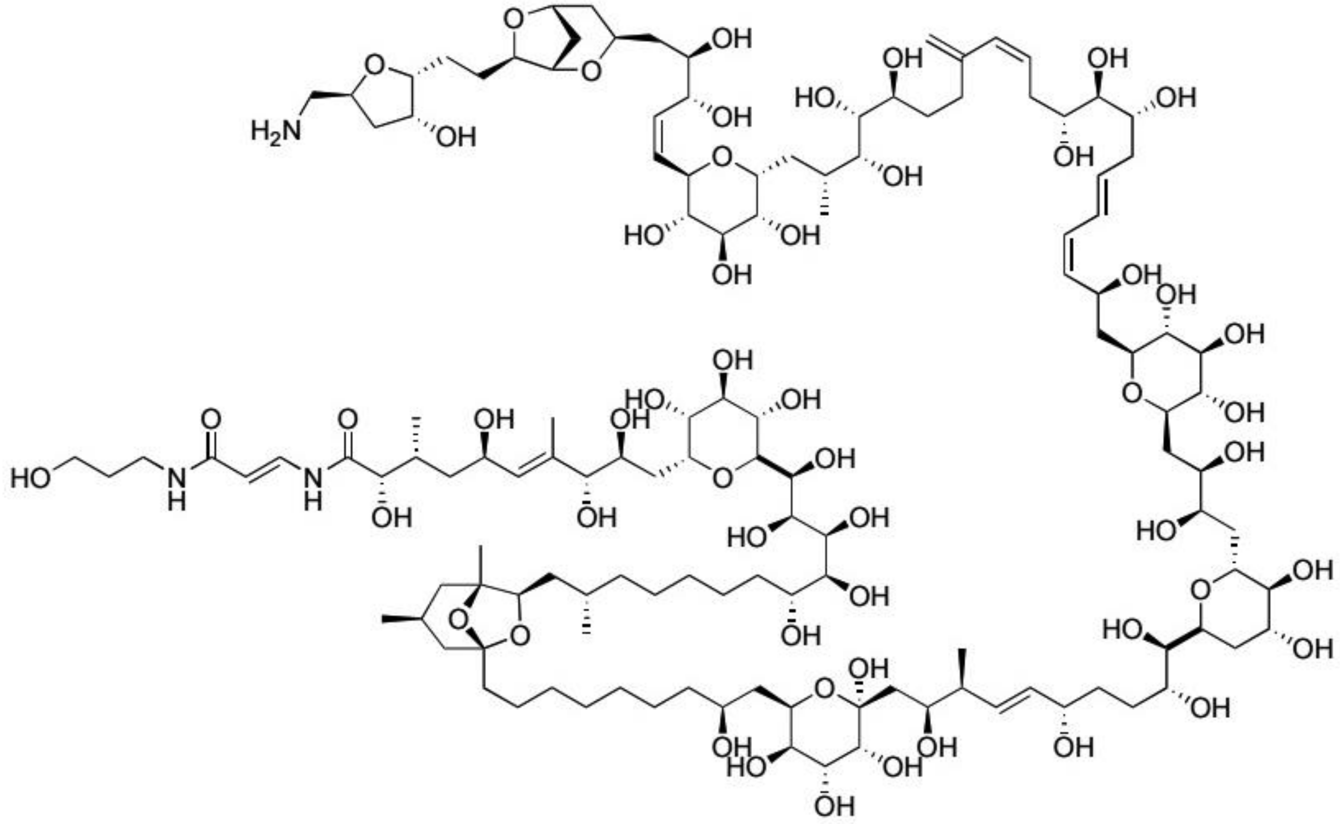


Omaezallene

(2*R*,3*S*,5*R*)-5-((*R*)-3-bromopropa-1,2-dien-1-yl)-2-((1*S*,2*S*,3*E*,5*E*)-1,6-dibromo-2-hydroxyocta-3,5-dien-1-yl)tetrahydrofuran-3-ol



Palytoxin



Palytoxin

(2S,3R,5R,8R,9S,E)-10-((2R,3R,4R,5S,6R)-6-((1S,2R,3S,4S,5R,11S)-12-((1R,3S,5S,7R)-5-((S)-9-((2R,3R,4R,5R,6S)-6-((2S,3S,6S,9R,10R,E)-10-((2S,4R,5S,6R)-6-((2R,3R)-4-((2R,3S,4R,5R,6S)-6-((2S,3Z,5E,8R,9S,10R,12Z,17S,18R,19R,20R)-21-((2R,3R,4R,5S,6R)-6-((3R,4R,Z)-5-((1S,3R,5R,7R)-7-(2-((2R,3R,5S)-5-(aminomethyl)-3-hydroxytetrahydrofuran-2-yl)ethyl)-2,6-dioxabicyclo[3.2.1]octan-3-yl)-3,4-dihydroxypent-1-en-1-yl)-3,4,5-trihydroxytetrahydro-2H-pyran-2-yl)-2,8,9,10,17,18,19-heptahydroxy-20-methyl-14-methylenehenicosa-3,5,12-trien-1-yl)-3,4,5-trihydroxytetrahydro-2H-pyran-2-yl)-2,3-dihydroxybutyl)-4,5-dihydroxytetrahydro-2H-pyran-2-yl)-2,6,9,10-tetrahydroxy-3-methyldec-4-en-1-yl)-3,4,5,6-tetrahydroxytetrahydro-2H-pyran-2-yl)-8-hydroxynonyl)-1,3-dimethyl-6,8-dioxabicyclo[3.2.1]octan-7-yl)-1,2,3,4,5-pentahydroxy-11-methyldodecyl)-3,4,5-trihydroxytetrahydro-2H-pyran-2-yl)-2,5,8,9-tetrahydroxy-N-((E)-3-((3-hydroxypropyl)amino)-3-oxoprop-1-en-1-yl)-3,7-dimethyldec-6-enamide

unique（ユニーク）/phonetic（電話で伝えられる）

文字	使用する語	文字	使用する語	文字	使用する語
A	Alpha	M	Mike	Y	Yankee
B	Bravo	N	November	Z	Zulu
C	Charlie	O	Oscar	0	Zero
D	Delta	P	Papa	1	One
E	Echo	Q	Quebec	2	Two
F	Foxtrot	R	Romeo	3	Three
G	Golf	S	Sierra	4	Four
H	Hotel	T	Tango	5	Five
I	India	U	Uniform	6	Six
J	Juliet	V	Victor	7	Seven
K	Kilo	W	Whiskey	8	Eight
L	Lima	X	X-Ray	9	Nine

文字	綴り	文字	綴り	文字	綴り	文字	綴り	文字	綴り
ア	朝日のア	イ	いろはのイ	ウ	上野のウ	エ	英語のエ	オ	大阪のオ
カ	為替のカ	キ	切手のキ	ク	クラブのク	ケ	景色のケ	コ	子供のコ
サ	桜のサ	シ	新聞のシ	ス	すずめのス	セ	世界のセ	ソ	そろばんのソ
タ	煙草のタ	チ	千鳥のチ	ツ	つるかめのツ	テ	手紙のテ	ト	東京のト
ナ	名古屋のナ	ニ	日本[1]のニ	ヌ	沼津のヌ	ネ	ねずみのネ	ノ	野原のノ
ハ	はがきのハ	ヒ	飛行機のヒ	フ	富士山のフ	ヘ	平和のヘ	ホ	保険のホ
マ	マッチのマ	ミ	三笠のミ	ム	無線のム	メ	明治のメ	モ	もみじのモ
ヤ	大和のヤ			ユ	弓矢のユ			ヨ	吉野のヨ
ラ	ラジオのラ	リ	りんごのリ	ル	留守居のル	レ	れんげのレ	ロ	ローマのロ
ワ	わらびのワ	ヰ	ゐどのヰ			ヱ	かぎのあるヱ	ヲ	尾張のヲ
ン	おしまいのン	゛	濁点	゜	半濁点				

identification

||

to be named reflecting structure
(unambiguous text)

titanium(IV) oxide = TiO_2

IUPAC recommendation on inorganic compounds

IR-11 Solid

IR-11.1.1 General

This chapter deals with some aspects of terminology, nomenclature and notation for (inorganic) solids. However, in cases where detailed structural information is to be conveyed, fully systematic names can be difficult to construct.

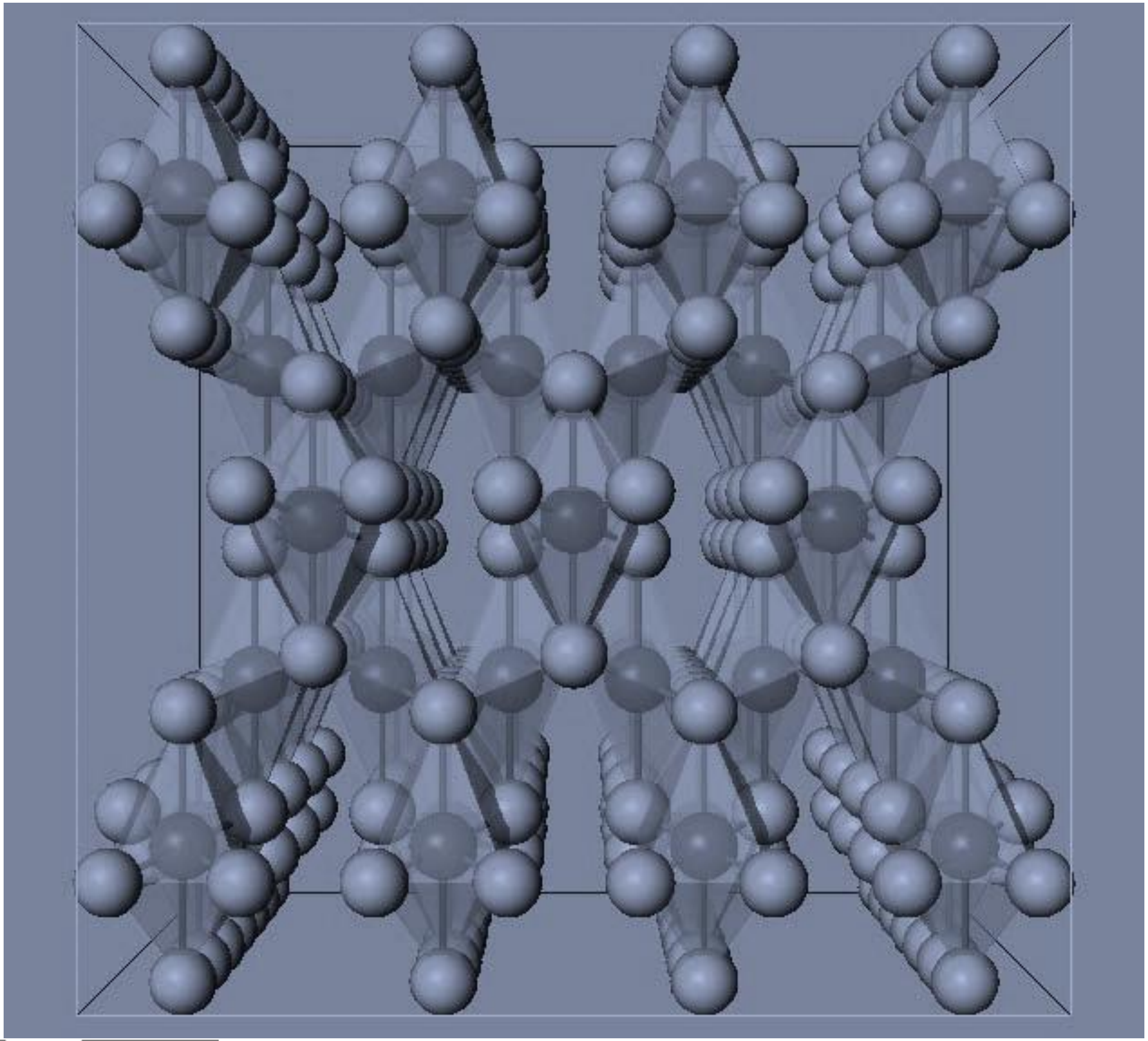
Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005, The Royal Society of Chemistry (2005) p. 236.

science/科学

unambiguousness + text

あいまいじゃない + ことばであらわす

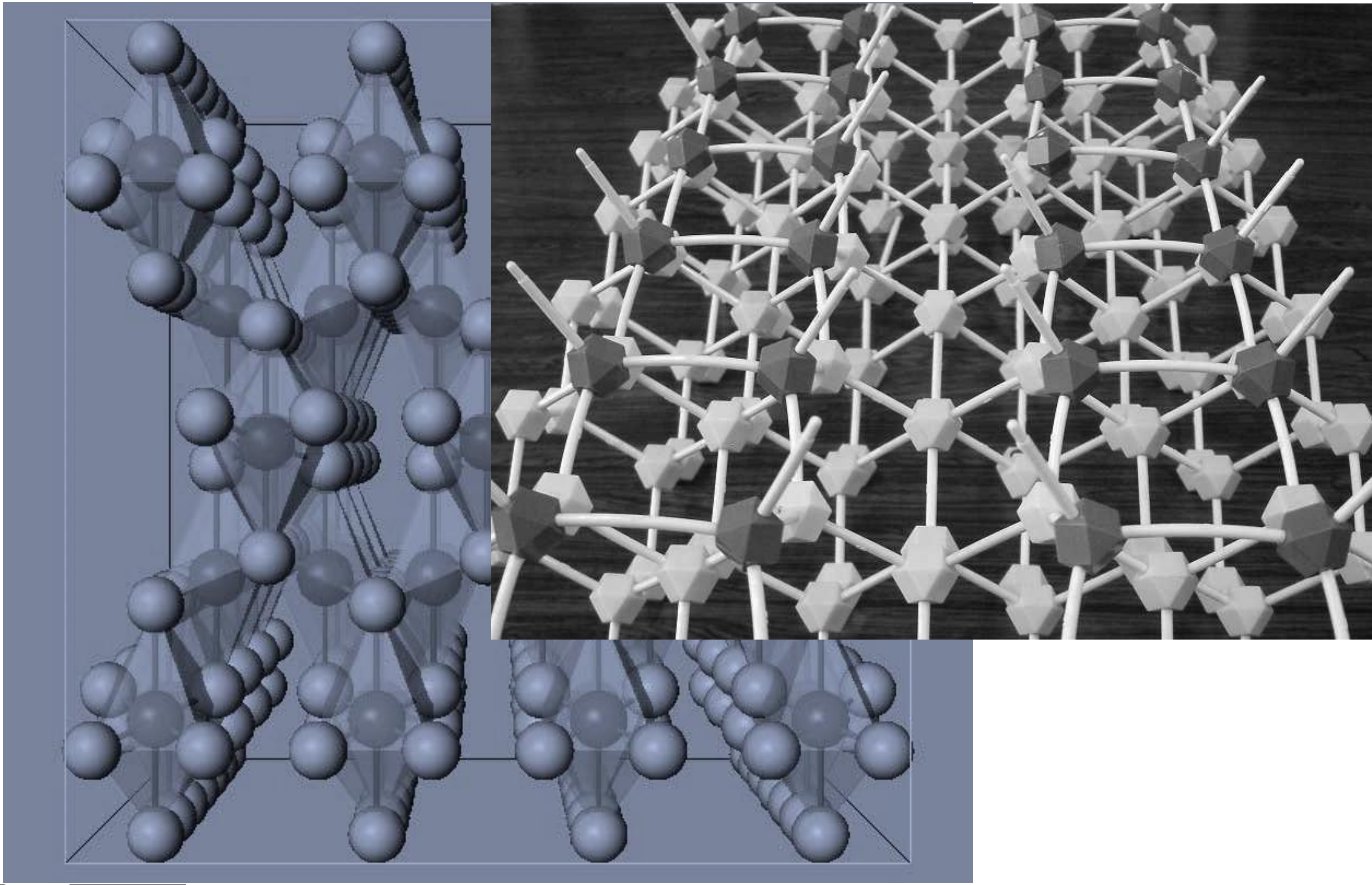
bulk (crystal lattice)



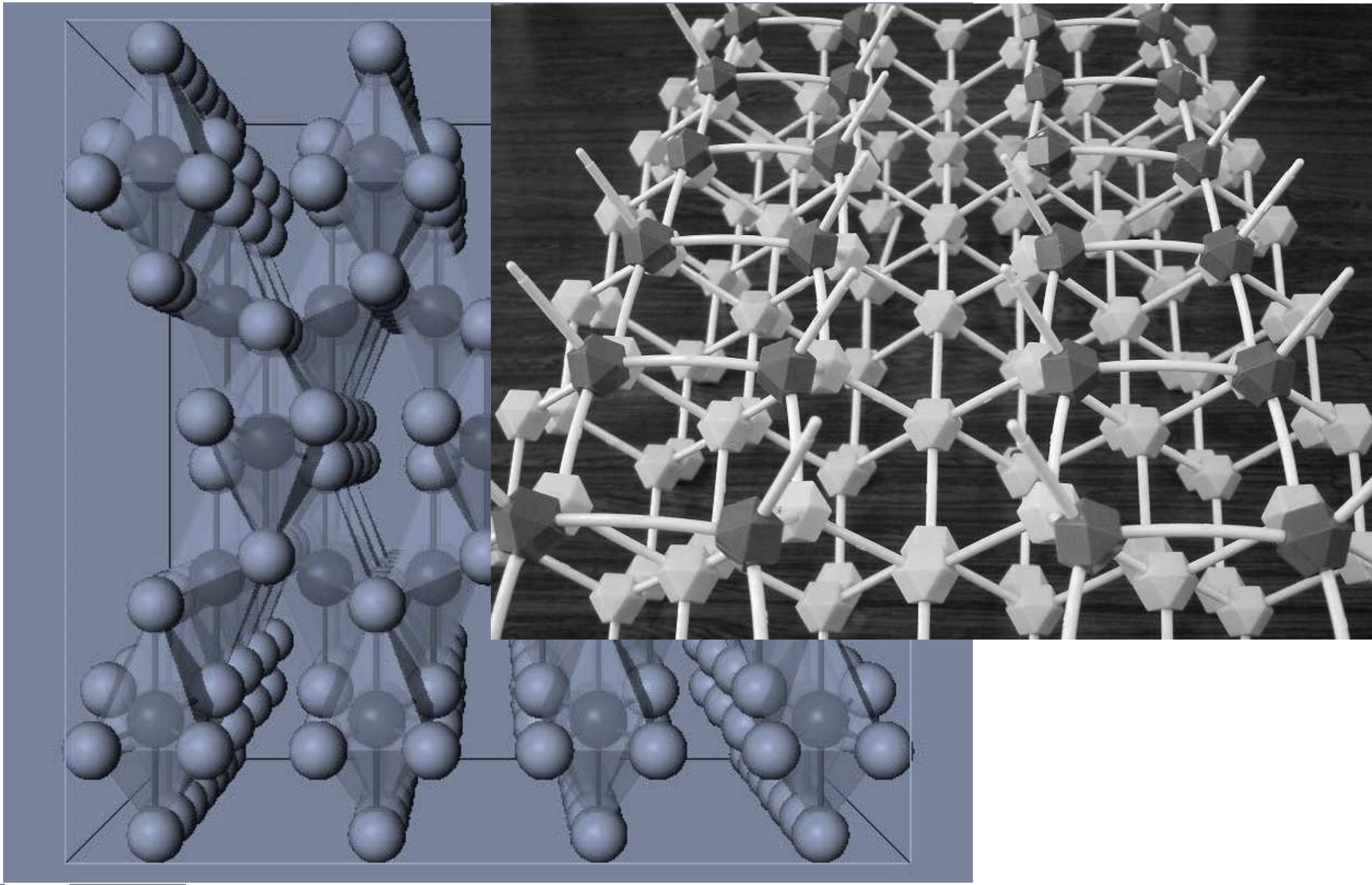
eTrap

bulk (crystal lattice)

surface



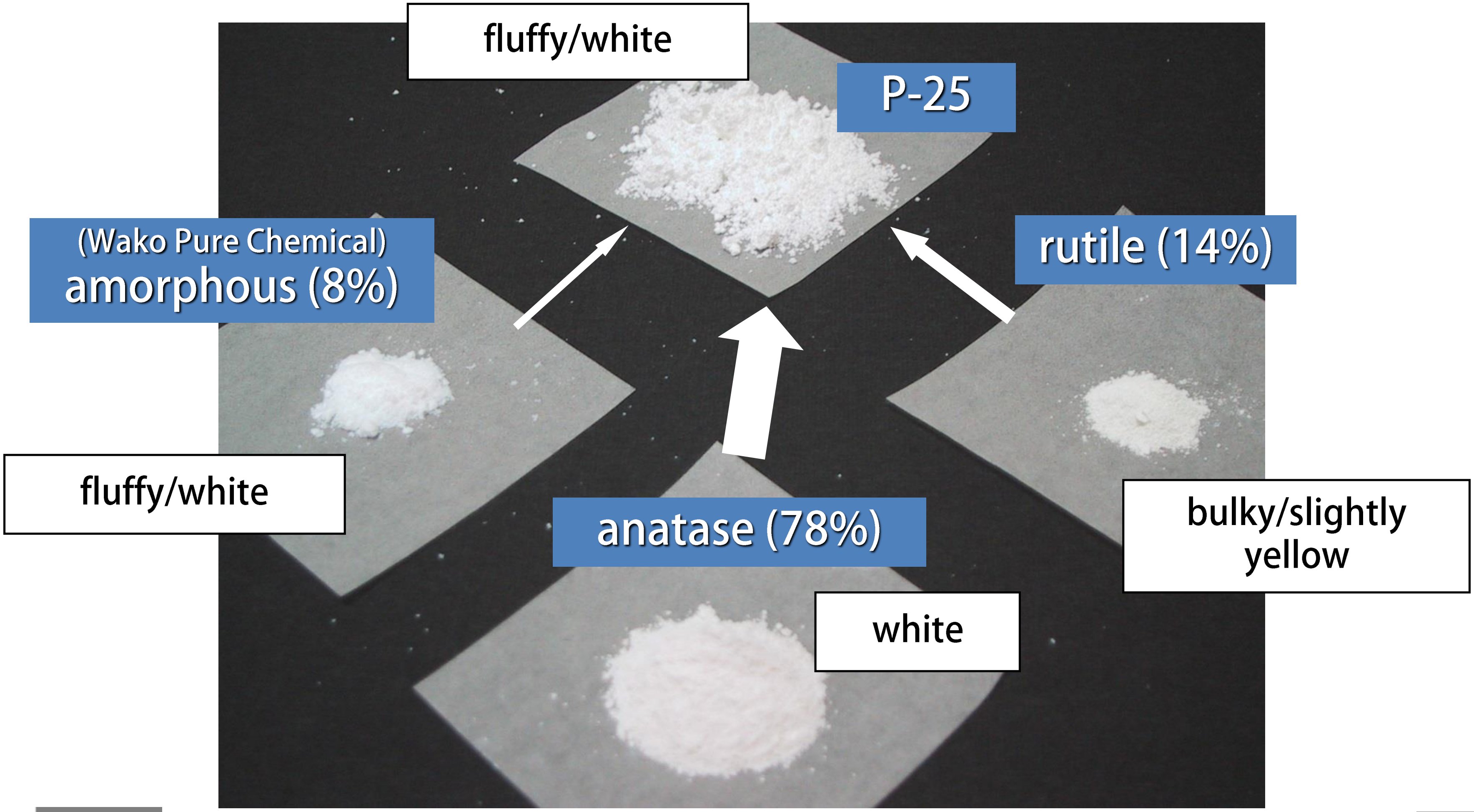
bulk (crystal lattice) <size> surface



eTrap

reconstruction of P25 from components

Ohtani, B.; Prieto-Mahaney, O.-O.; Li, D.; Abe, R. *J. Photochem. Photobiol. A Chem.* **2010**, *216*, 179-182. [178]



inhomogeneous composition of P25

Ohtani, B.; Prieto-Mahaney, O.-O.; Li, D.; Abe, R. *J. Photochem. Photobiol. A Chem.* **2010**, *216*, 179-182. [178]

- sample supplied in "1-kg package"
- re-packed in several bottles
- sampling ... how? top/middle/bottom

crystal composition depending on the collection point

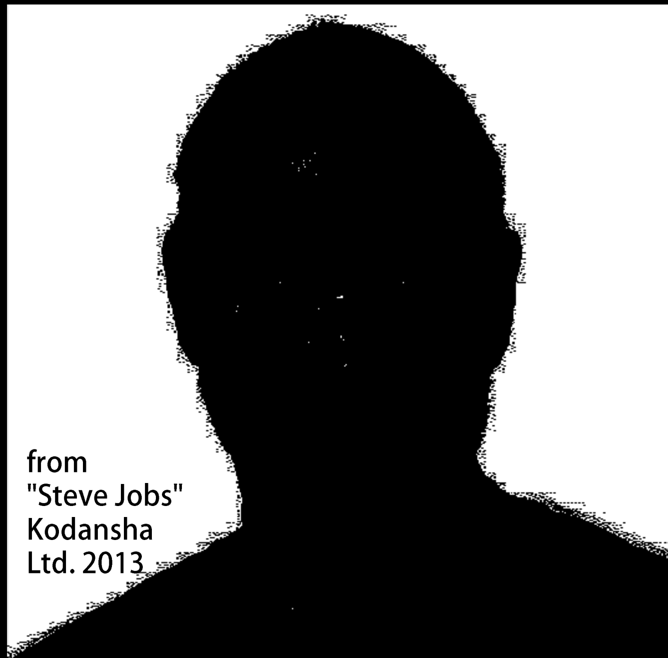
- presumably due to anatase, rutile and amorphous domains are produced in the "flame-synthesis" procedure

- no guarantee for:

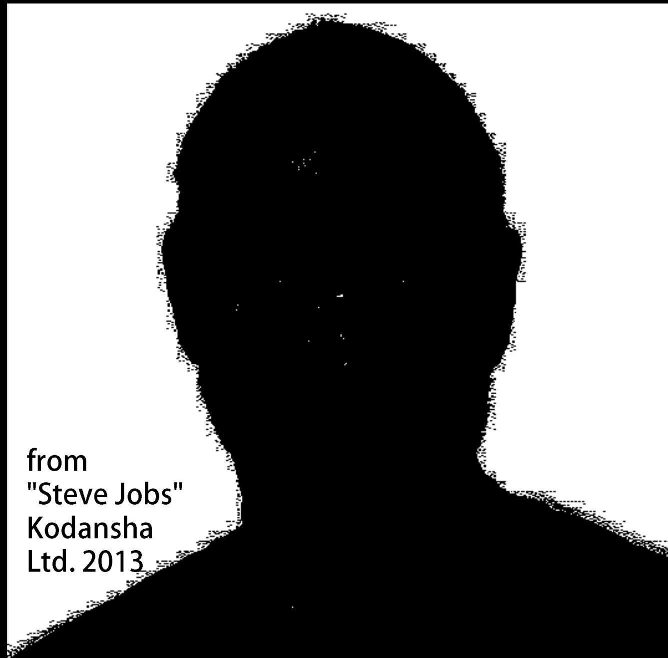
samples taken from the same bottle has 78:14:8 ratio

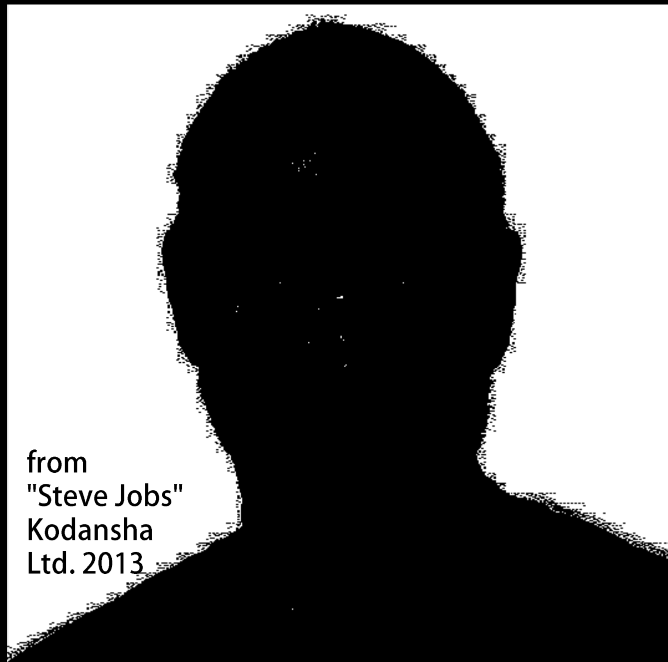
your P25 sample has the crystal content of 78:14:8.

crystalline phase
primary particle size
secondary particle size
specific surface area

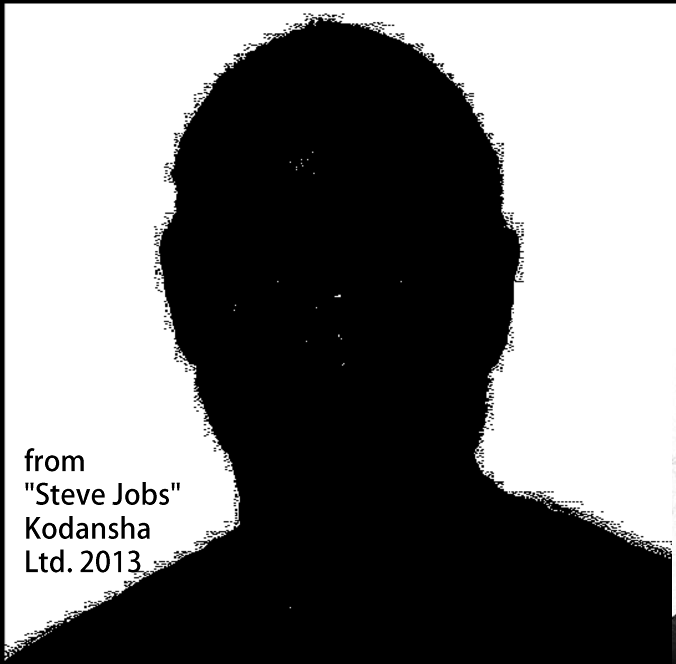


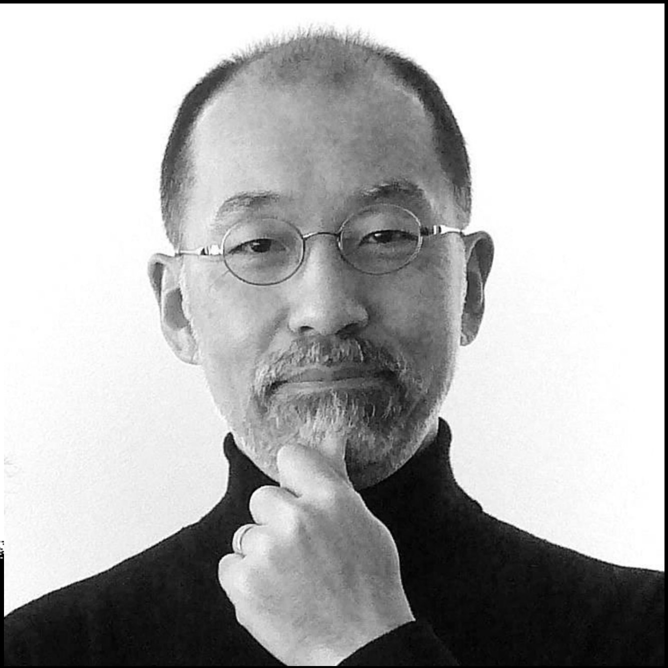
from
"Steve Jobs"
Kodansha
Ltd. 2013


from
"Steve Jobs"
Kodansha
Ltd. 2013



(thin) hair
wire-frame glasses
(gray) beard and mustache
ring on left third (ring) finger
black turtle-neck sweater
handsome!





(thin) hair
wire-frame glasses
(gray) beard and mustache
ring on left third (ring) finger
black turtle-neck sweater
handsome!
fingerprint

crystalline phase
primary particle size
secondary particle size
specific surface area

crystalline phase
primary particle size
secondary particle size
specific surface area

ERDT/CBB pattern

energy-resolved density of electron-traps (ERDT)/conduction-band bottom (CBB)

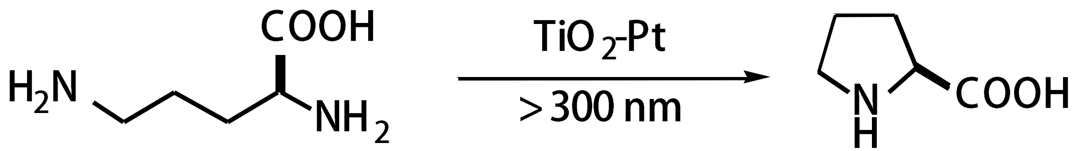
as a

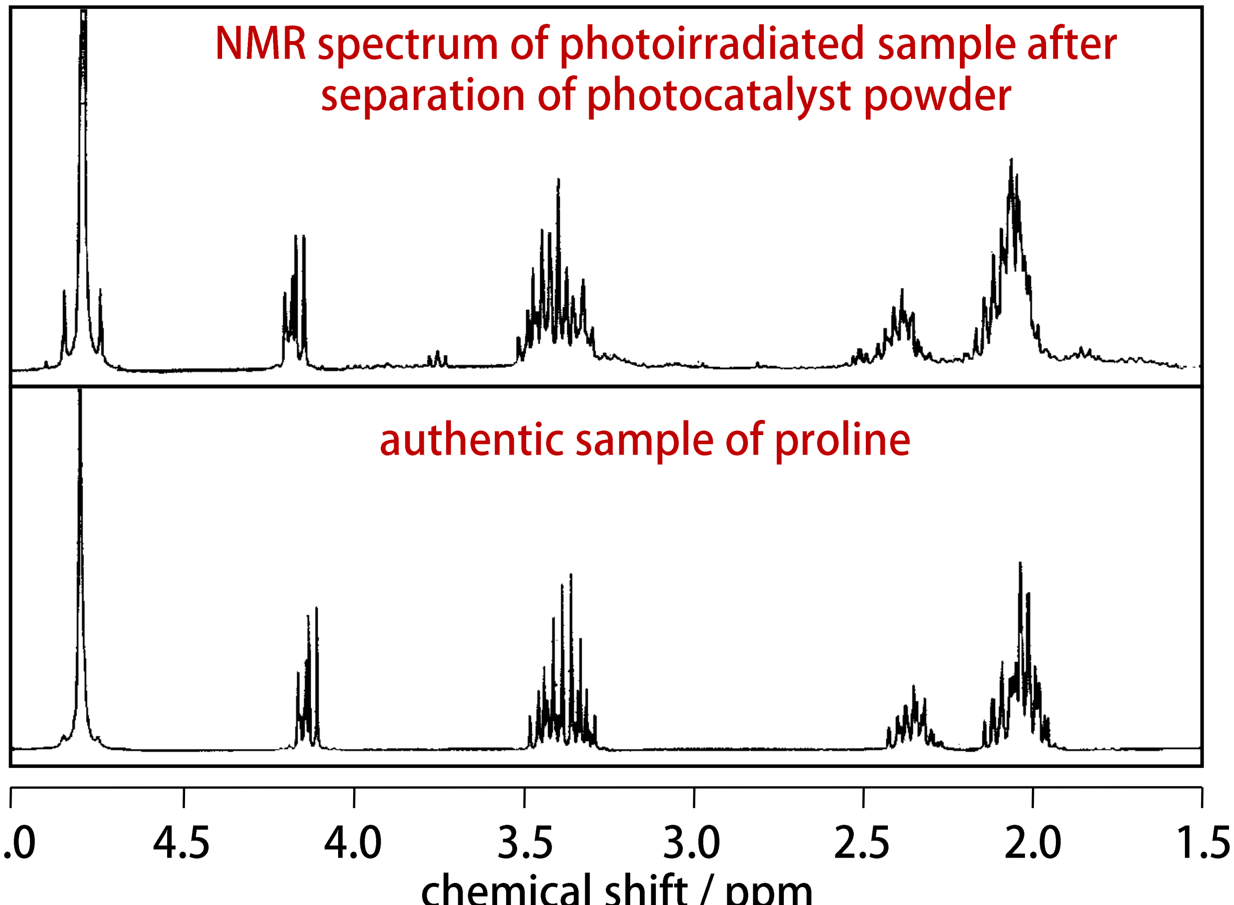
finger print

for identification of metal-oxide powders

identification of organic compounds

Ohtani, B.; Tsuru, S.; Nishimoto, S.-i.; Kagiya, T.; Izawa, K. *J. Org. Chem.* **1990**, *55*, 5551-5553. [64]

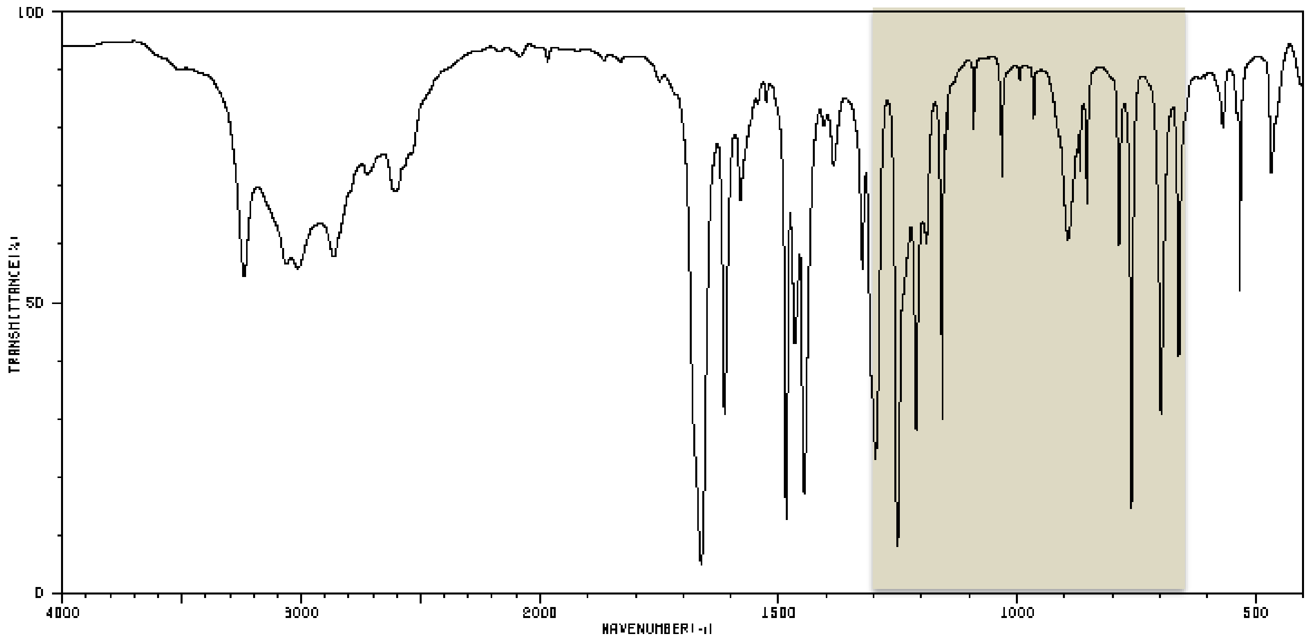




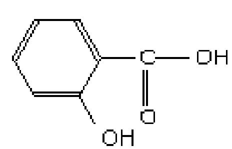
infrared absorption spectroscopy

✓ 650～1300 cm^{-1} = fingerprint region

HIT-NO=1330	SCORE= ( )	SDBS-NO=1149	IR-NIDA-08453 : KBR DISC
SALICYLIC ACID			
$C_7H_6O_3$			

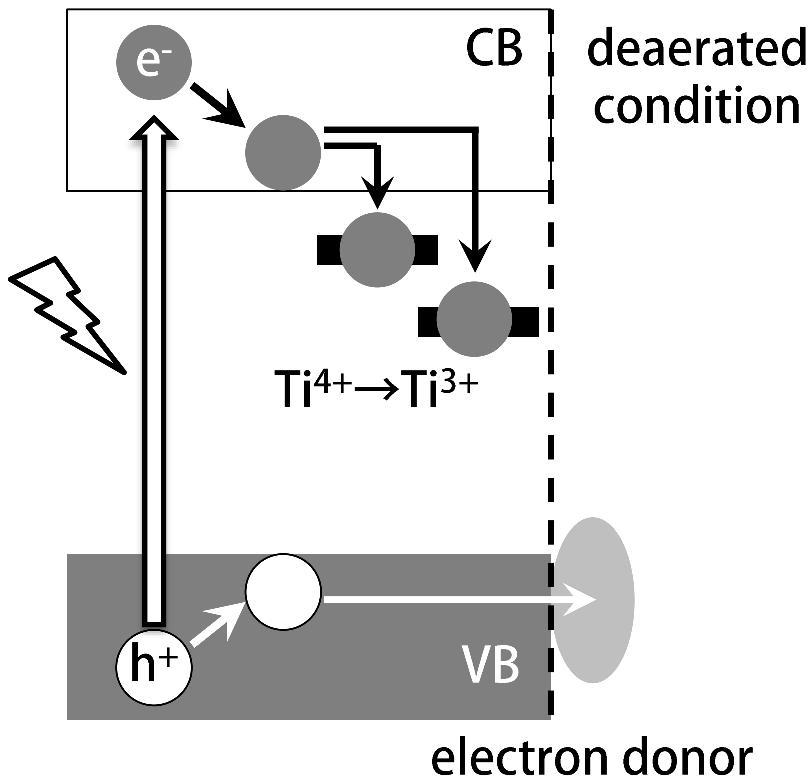


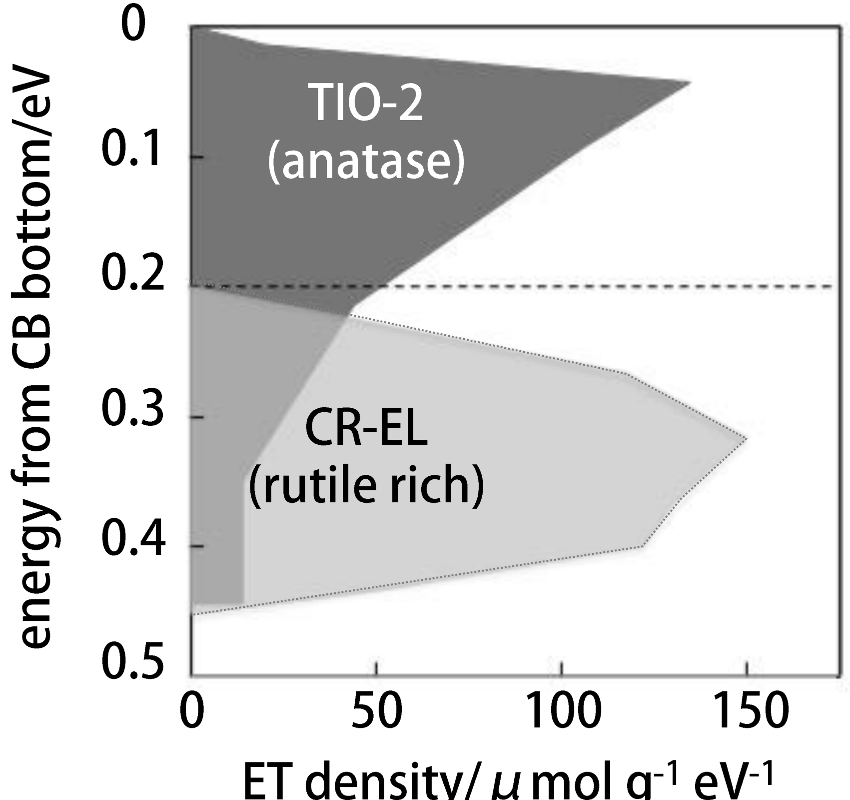
3240	62	1680	64	1326	63	1161	72	786	67
3013	53	1527	81	1297	21	1091	77	760	13
2864	55	1484	12	1251	7	1032	68	699	29
2724	70	1467	41	1239	49	966	79	661	38
2605	66	1447	16	1212	26	893	58	569	77
1662	4	1405	77	1190	58	868	70	533	50
1613	29	1386	70	1167	28	863	64	467	70



photochemical method for ERDT measurement

Ikeda, S.; Sugiyama, N.; Murakami, S.-y.; Kominami, H.; Kera, Y.; Noguchi, H.; Uosaki, K.; Torimoto, T.; Ohtani, B. *Phys. Chem. Chem. Phys.* **2003**, *5*, 778-783. [118]

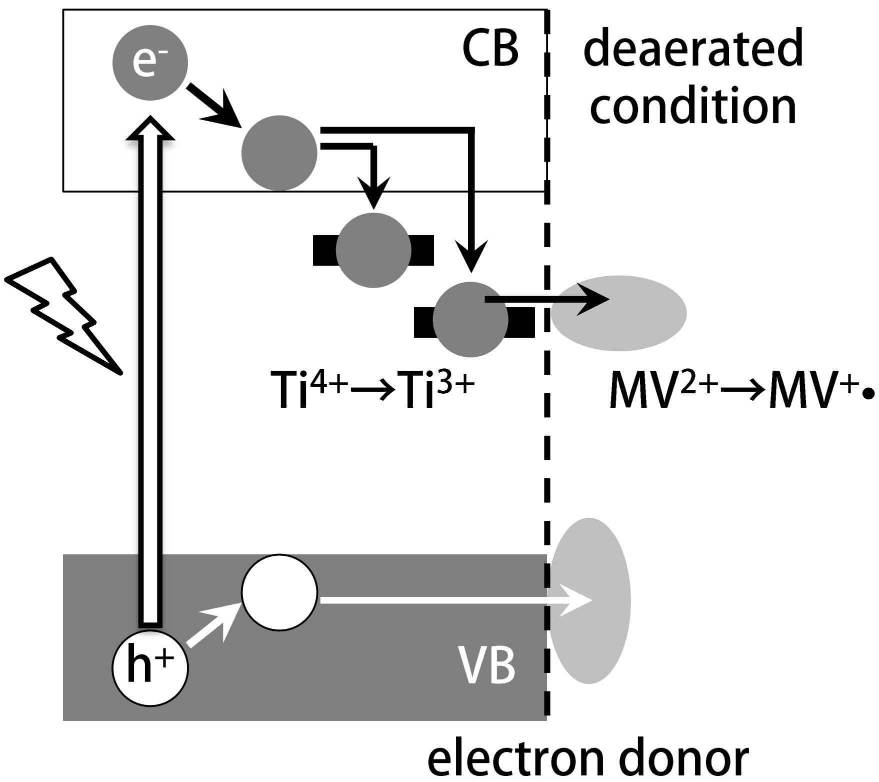


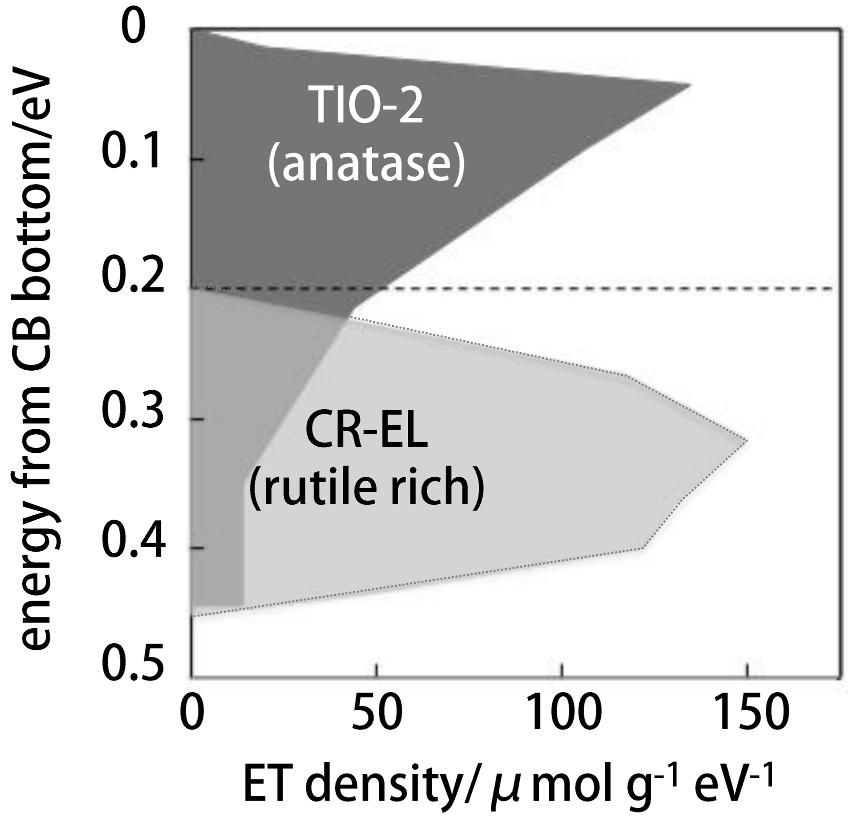


- low energy resolution
- limitation of trap-energy range

photochemical method for ERDT measurement

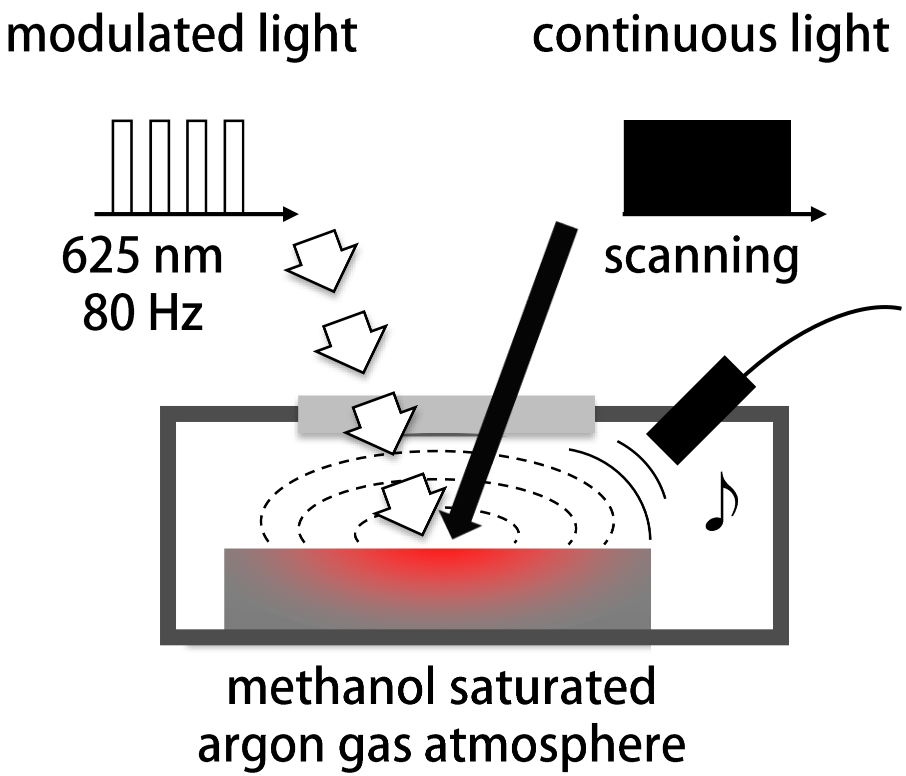
Ikeda, S.; Sugiyama, N.; Murakami, S.-y.; Kominami, H.; Kera, Y.; Noguchi, H.; Uosaki, K.; Torimoto, T.; Ohtani, B. *Phys. Chem. Chem. Phys.* **2003**, *5*, 778-783. [118]

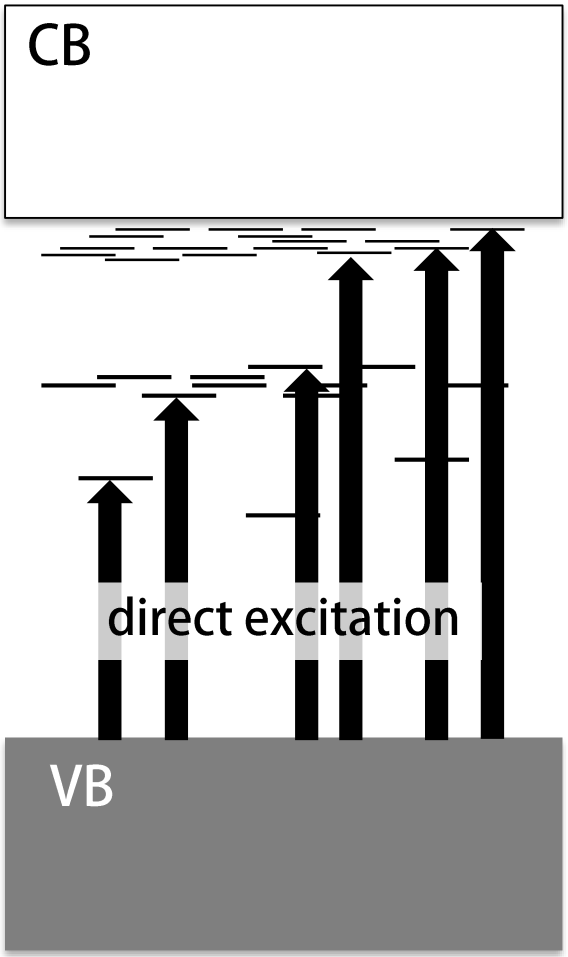




- ➢ low energy resolution
- ➢ limitation of trap-energy range

reversed double-beam photoacoustic spectroscopy (RDB-PAS)

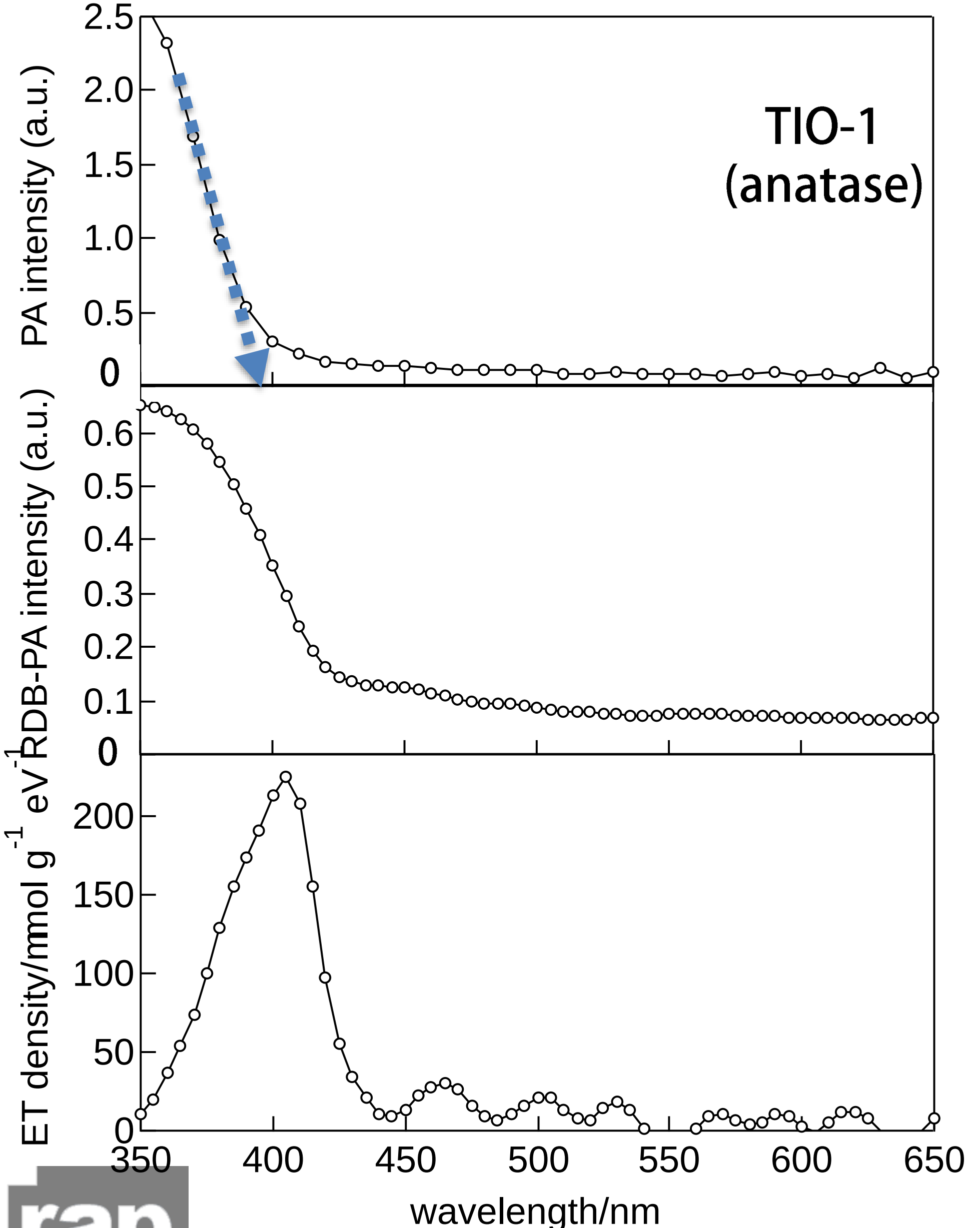


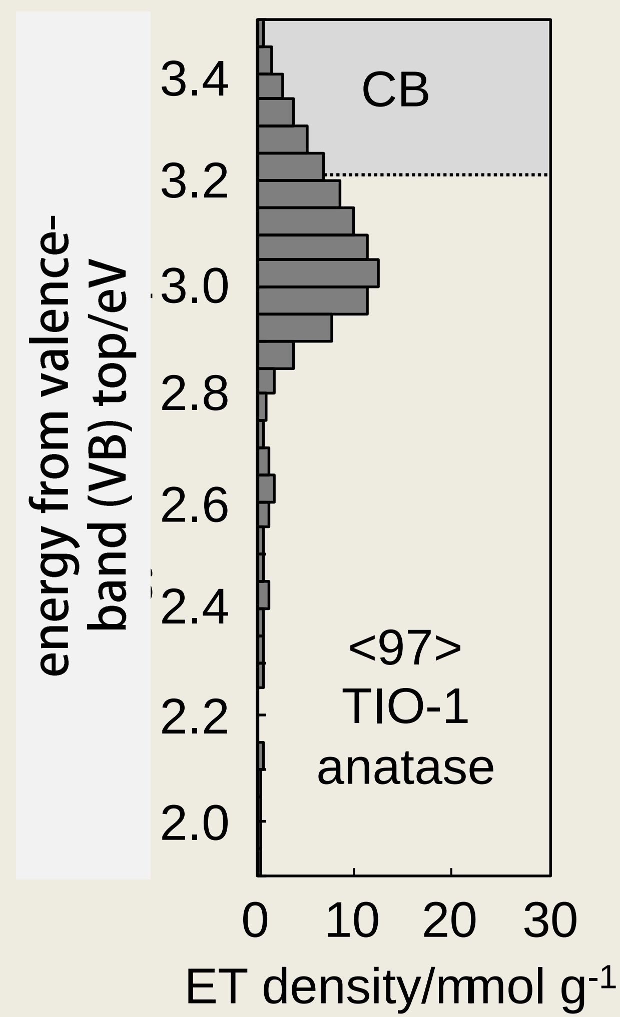


filling electron traps selectively from deeper side

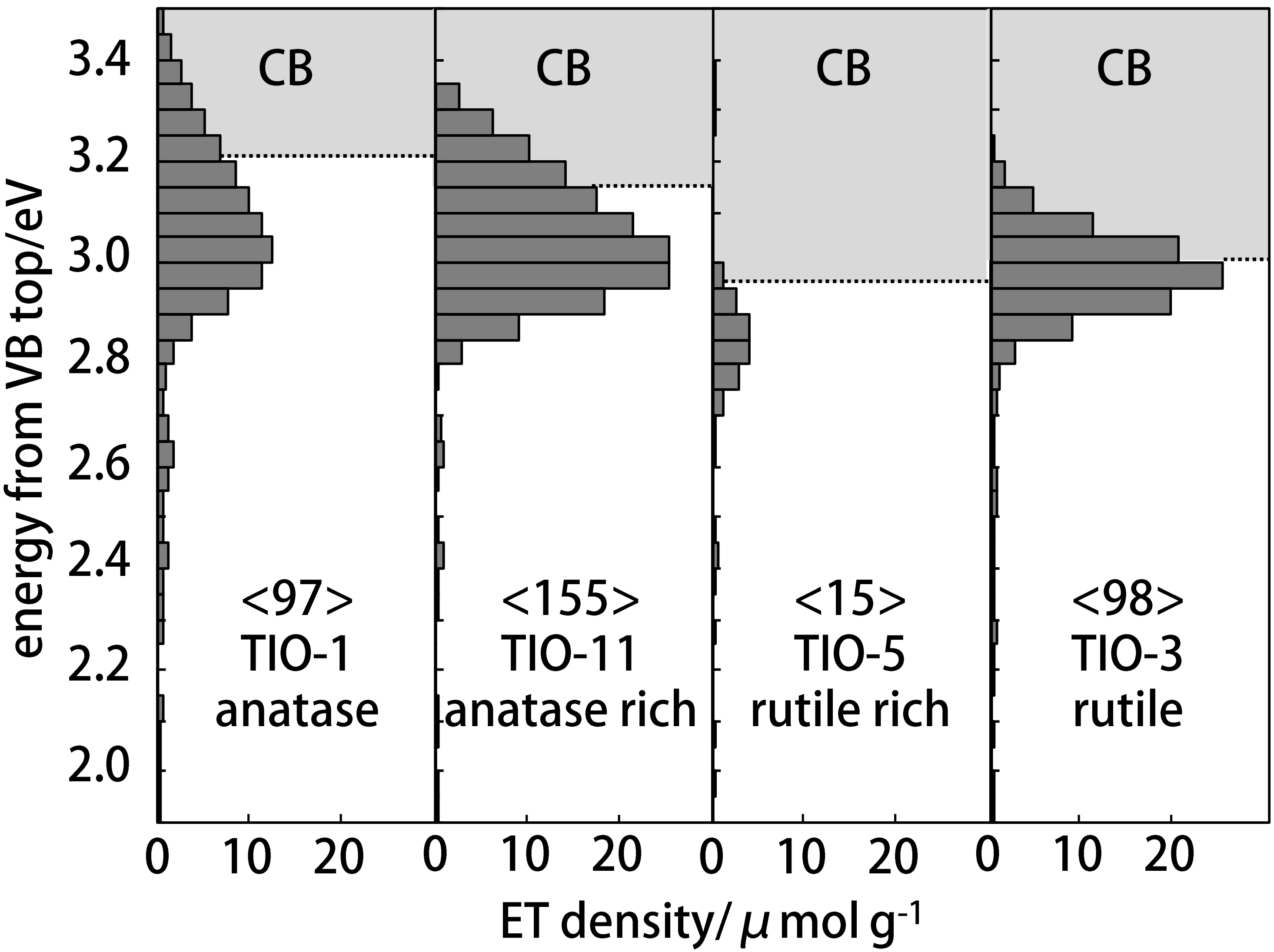

BNC出力
OFF
DCジャック出力

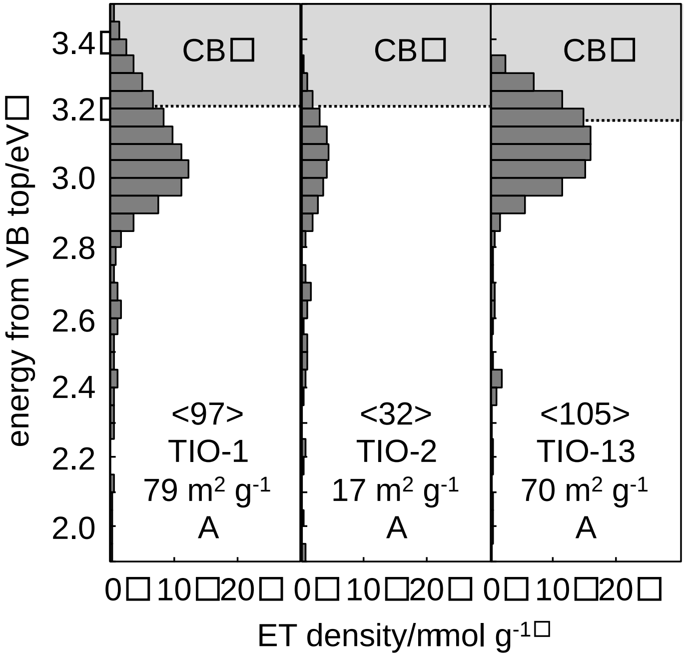
reversed double-beam photoacoustic spectroscopy (RDB-PAS)

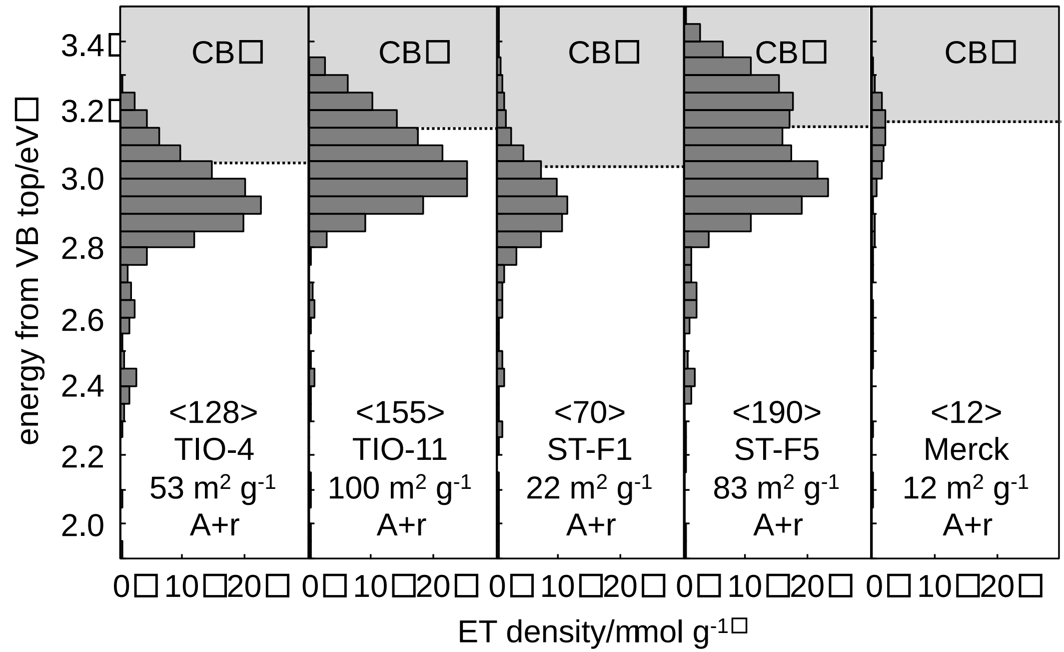


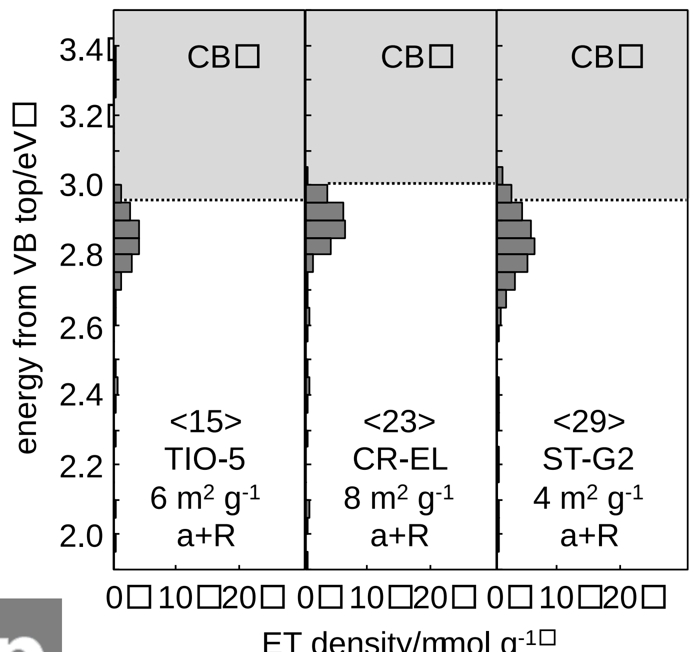


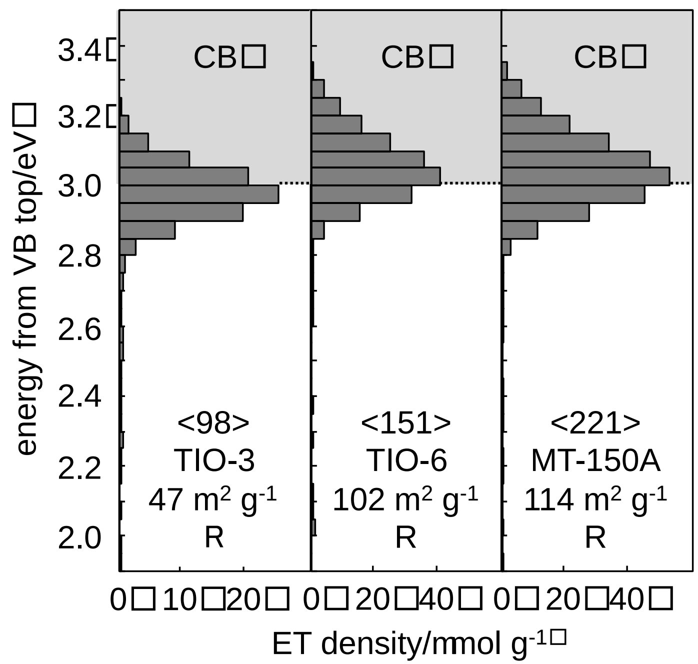
e-trap

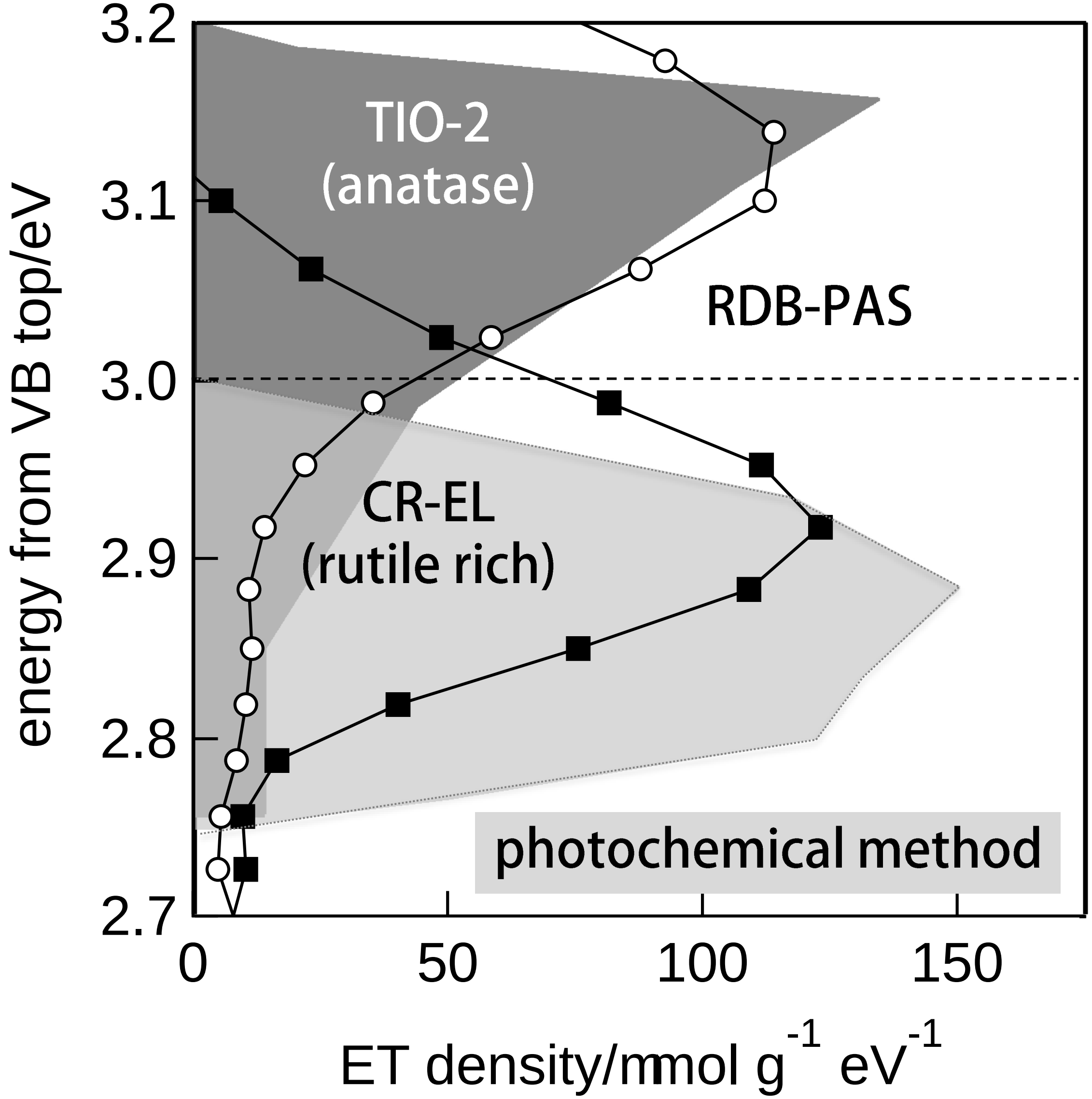

CB
CB
CB
CB
<97>
TIO-1
anatase
<155>
TIO-11
anatase rich
<15>
TIO-5
rutile rich
<98>
TIO-3
rutile
energy from VB top/eV
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
0
10
20
ET density/ μ mol g-1


energy from VB top/eV
CB
<97> TIO-1 79 m^2 g^{-1} A
<32> TIO-2 17 m^2 g^{-1} A
<105> TIO-13 70 m^2 g^{-1} A
ET density/mmol g^{-1}


energy from VB top/eV
CB
<128> TIO-4 53 m^2 g^{-1} A+r
<155> TIO-11 100 m^2 g^{-1} A+r
<70> ST-F1 22 m^2 g^{-1} A+r
<190> ST-F5 83 m^2 g^{-1} A+r
<12> Merck 12 m^2 g^{-1} A+r
ET density/mmol g^{-1}

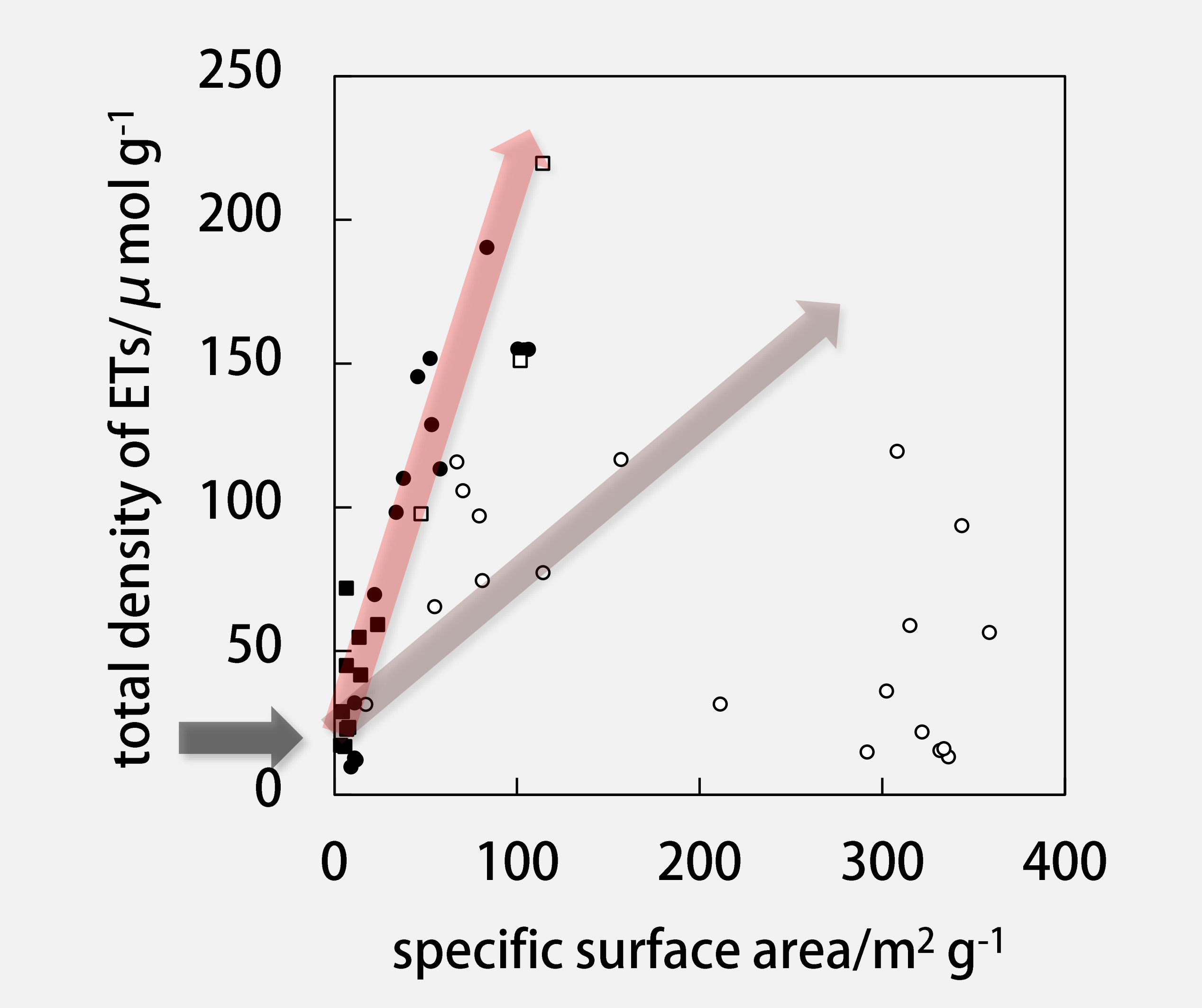

energy from VB top/eV
CB
<15> TIO-5 6 m^2 g^{-1} a+R
<23> CR-EL 8 m^2 g^{-1} a+R
<29> ST-G2 4 m^2 g^{-1} a+R
ET density/mmol g^{-1}


energy from VB top/eV
CB
<98> TIO-3 47 m^2 g^{-1} R
<151> TIO-6 102 m^2 g^{-1} R
<221> MT-150A 114 m^2 g^{-1} R
ET density/mmol g^{-1}



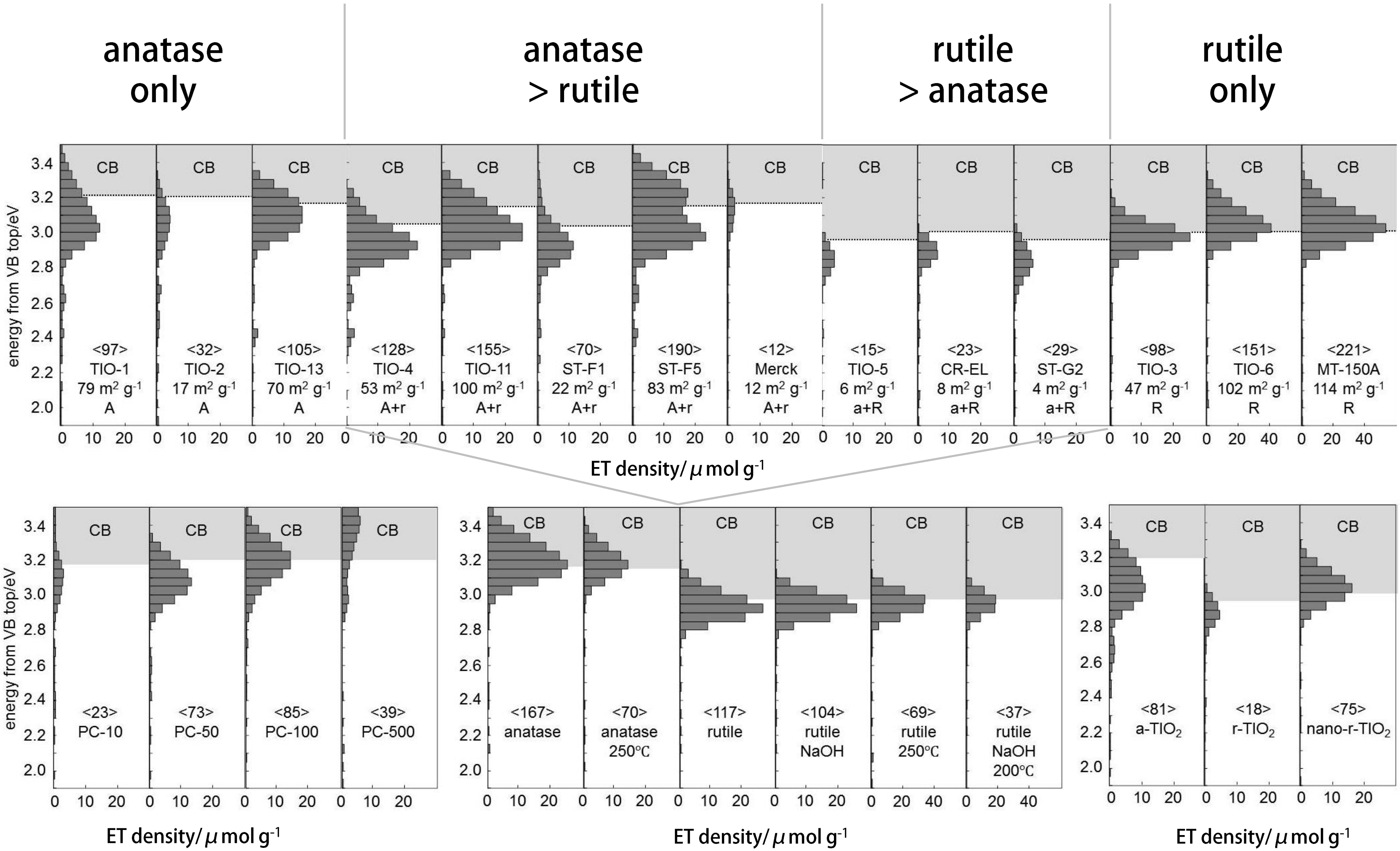
higher energy resolution and wider energy range

○ anatase, ● anatase rich, ■ rutile rich, □ rutile



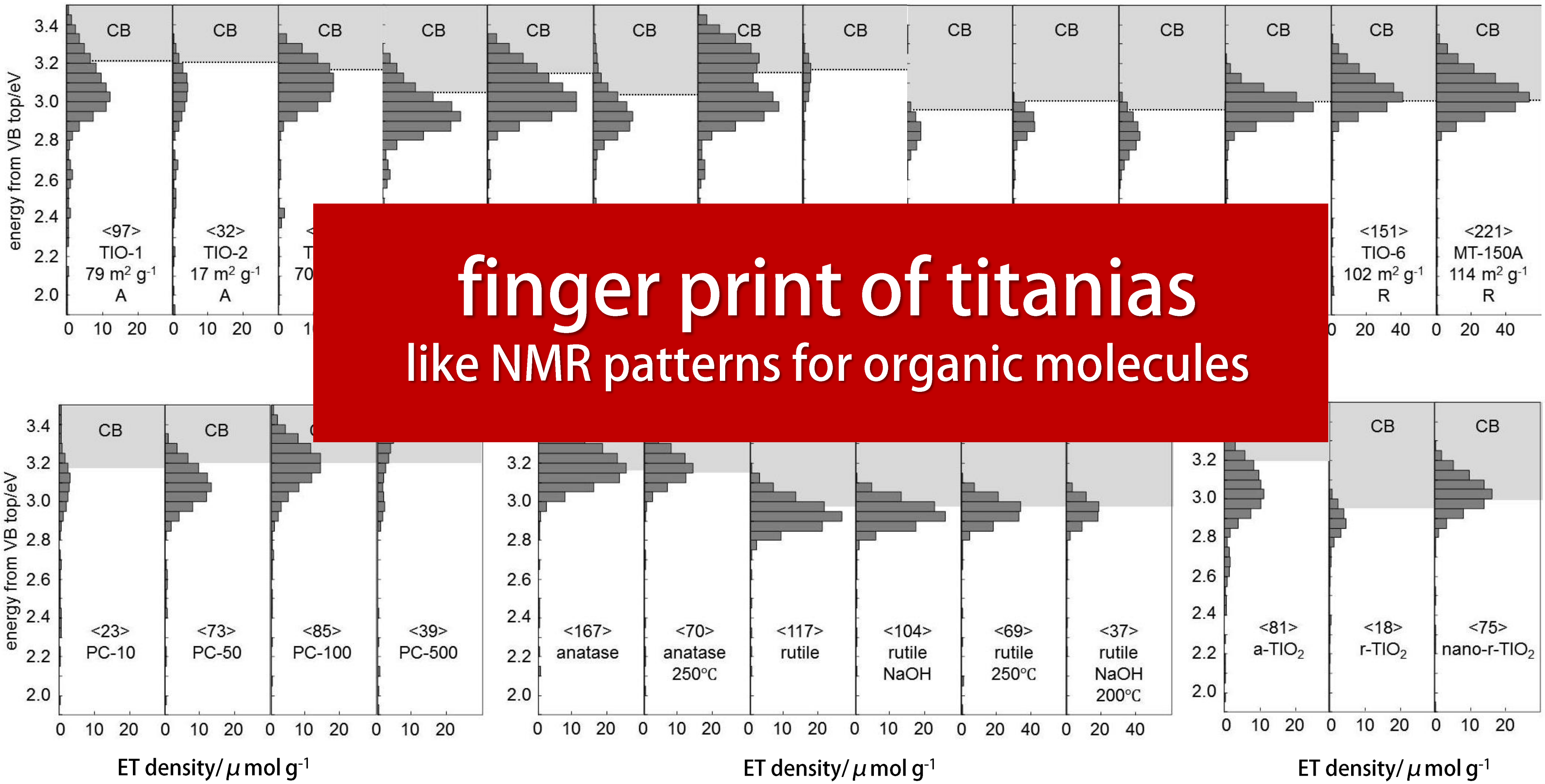
surface >> crystalline bulk

ERDT: energy-resolved distribution of traps



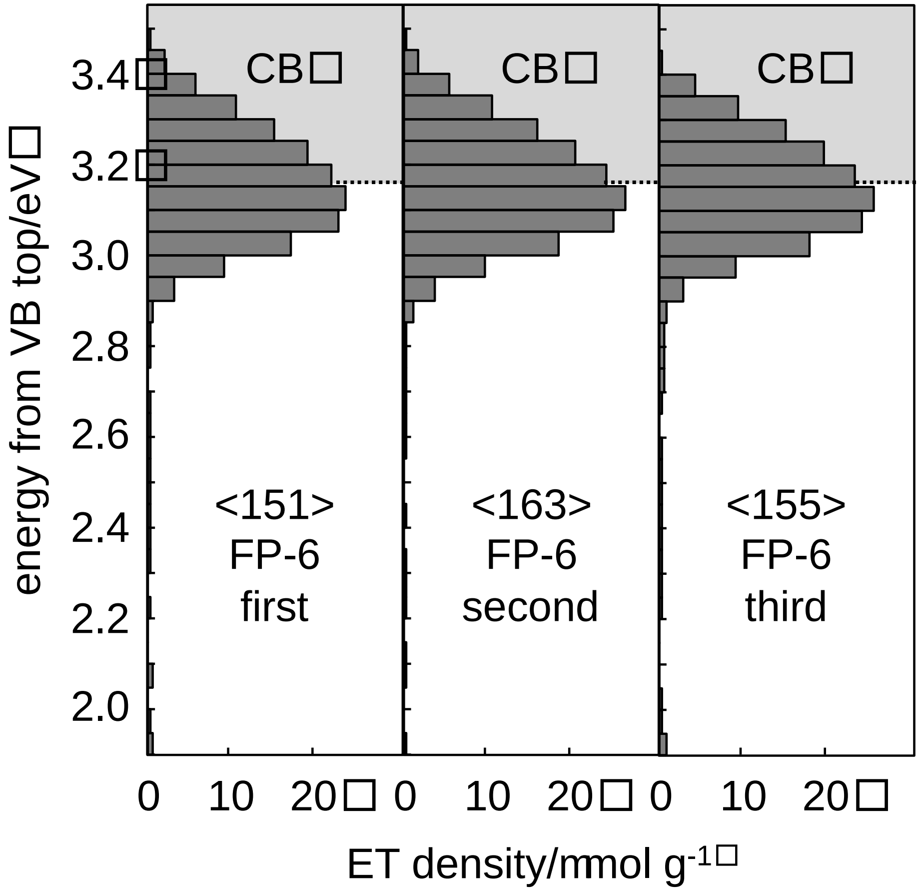
ERDT: energy-resolved distribution of traps

anatase only	anatase > rutile	rutile > anatase	rutile only



finger print of titanias

like NMR patterns for organic molecules



ζ(a): ERDT-pattern matching (f)

$$= 1 - \left(\int f(1) - \alpha f(2) \,/\, f(1) \right)$$

$$\alpha = \int \left(f(1) - \alpha f(2) \right)^2$$

$$\int f(1) < \int f(2)$$

ζ(b): total density of ETs (D)

$$= D(1) \,/\, D(2) \qquad [D(1) \leq D(2)]$$

ζ(c): CB bottom position (CBB)

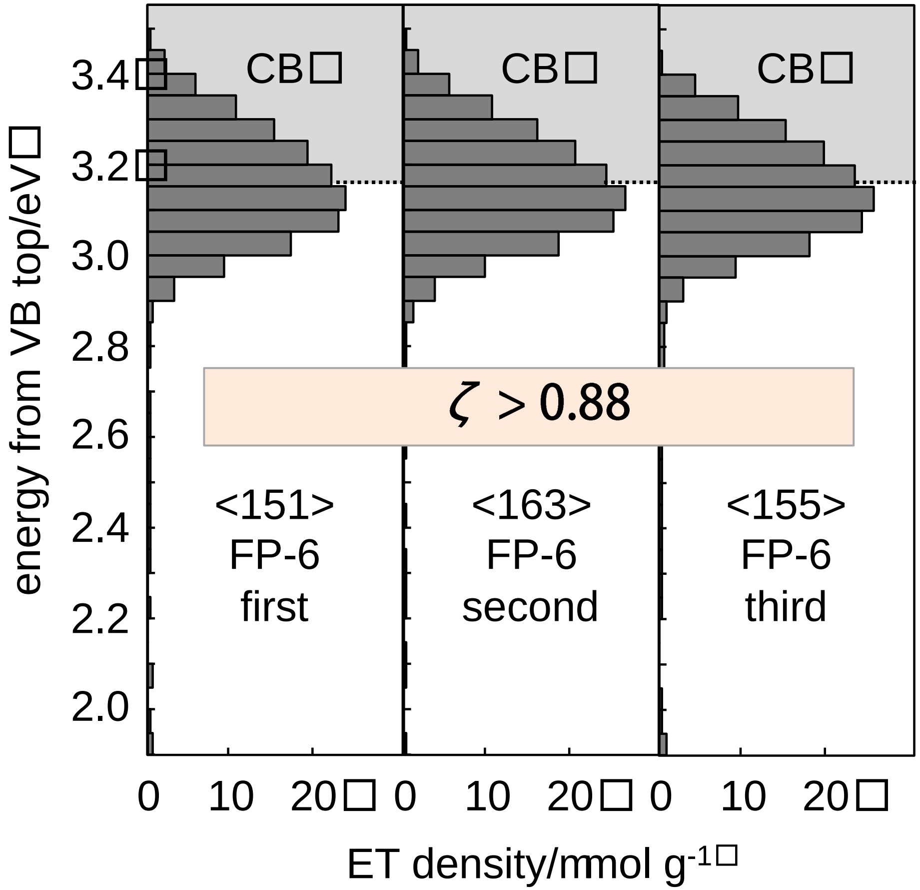
$$= CBB(1) \,/\, CBB(2)$$

$$[CBB(1) < CBB(2)]$$

standard deviation for degree of coincidence (ζ)

z(a)	z(b)	z(c)	z
0.0116	0.0185	0.000119	0.0145

$$\zeta = \zeta(a) \times \zeta(b)^{1/2} \times \zeta(c)^2$$



ζ(a): ERDT-pattern matching (f)

$$= 1 - (\int f(1) - \alpha f(2) / f(1))$$

$$\alpha = \int (f(1) - \alpha f(2))^2$$

$$\int f(1) < \int f(2)$$

ζ(b): total density of ETs (D)

$$= D(1) / D(2) \quad [D(1) \leq D(2)]$$

ζ(c): CB bottom position (CBB)

$$= CBB(1) / CBB(2)$$

$$[CBB(1) < CBB(2)]$$

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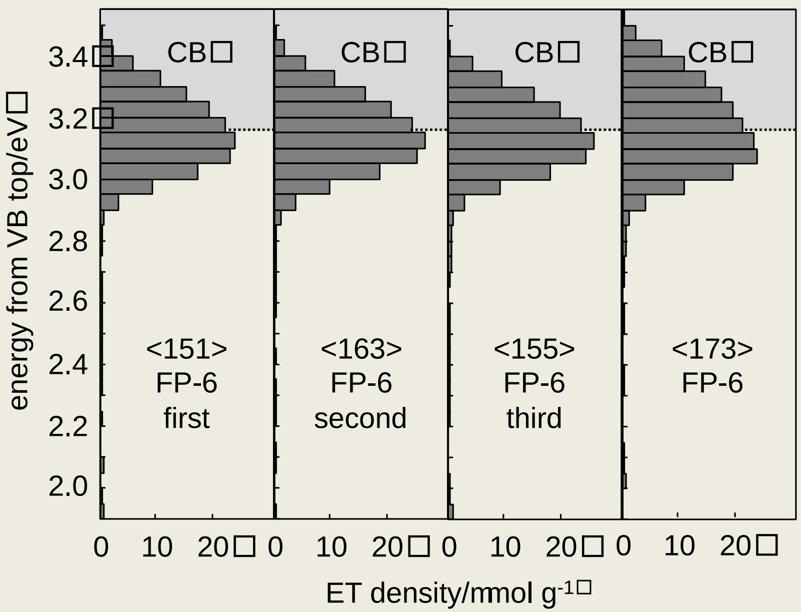
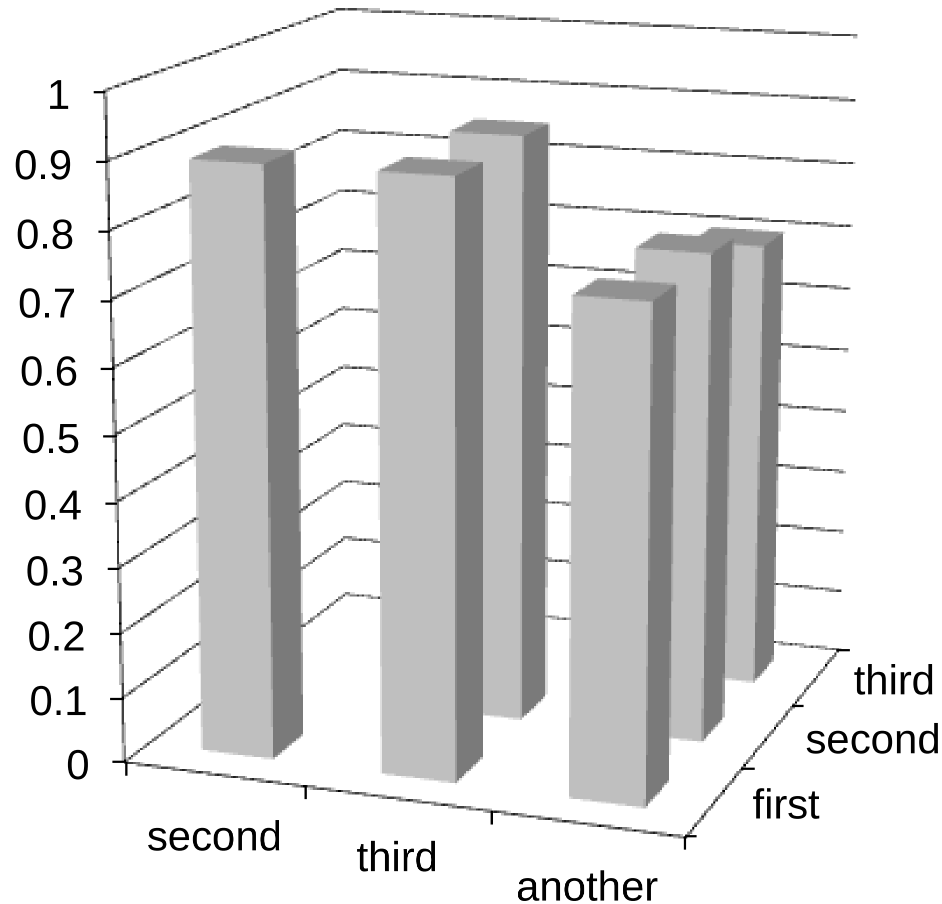
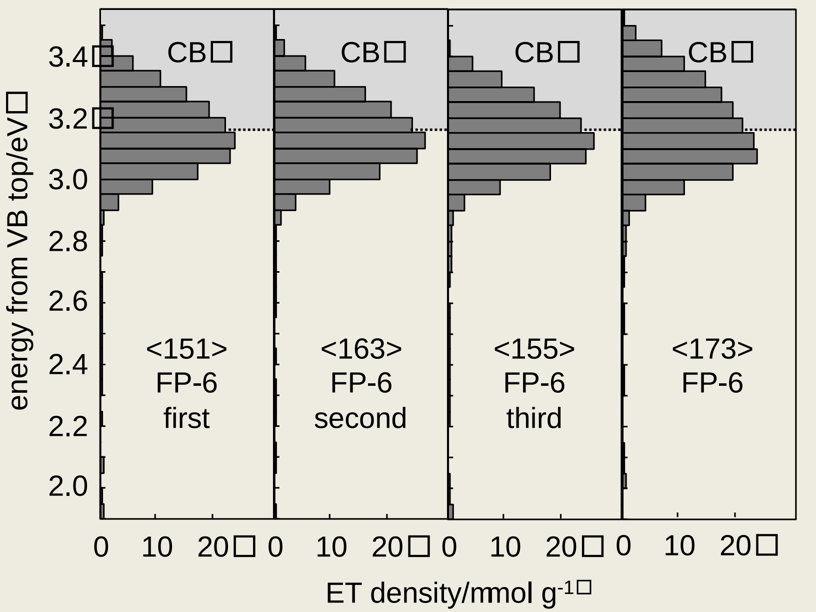
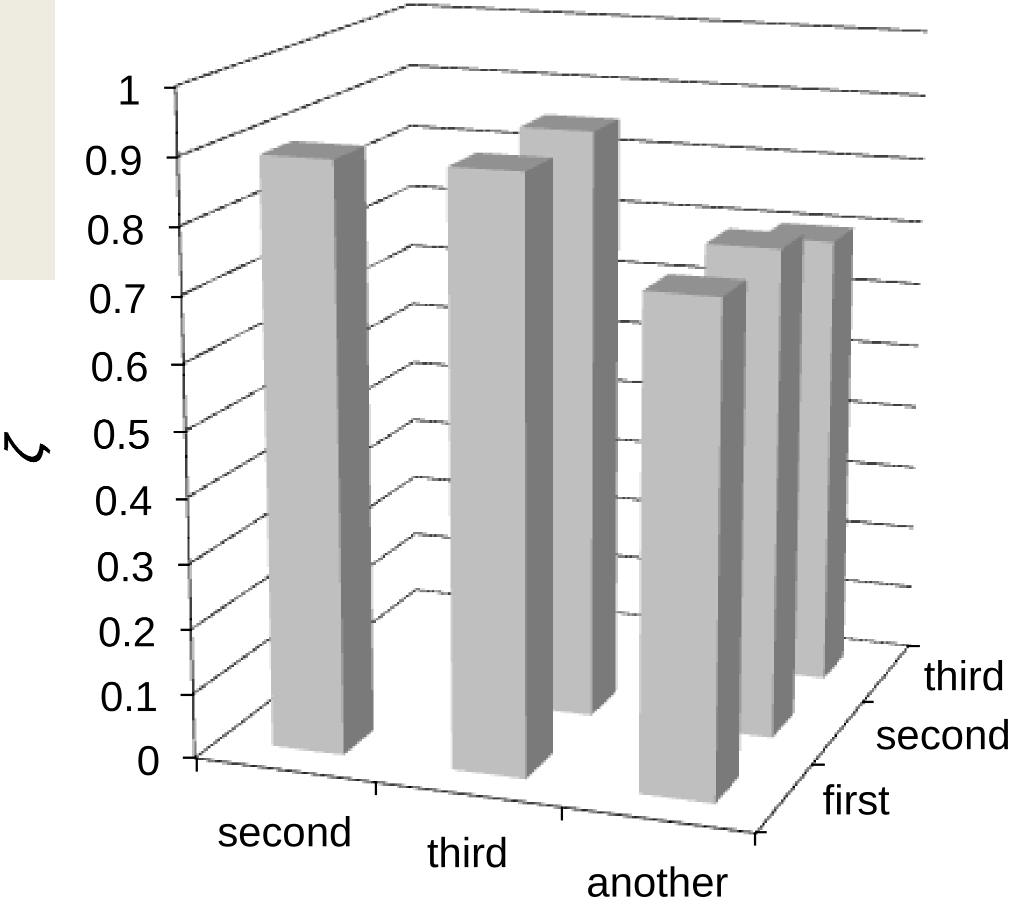

CB
CB
CB
CB
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
energy from VB top/eV
<151>
FP-6
first
<163>
FP-6
second
<155>
FP-6
third
<173>
FP-6
0 10 20 0 10 20 0 10 20 0 10 20
ET density/mmol g-1

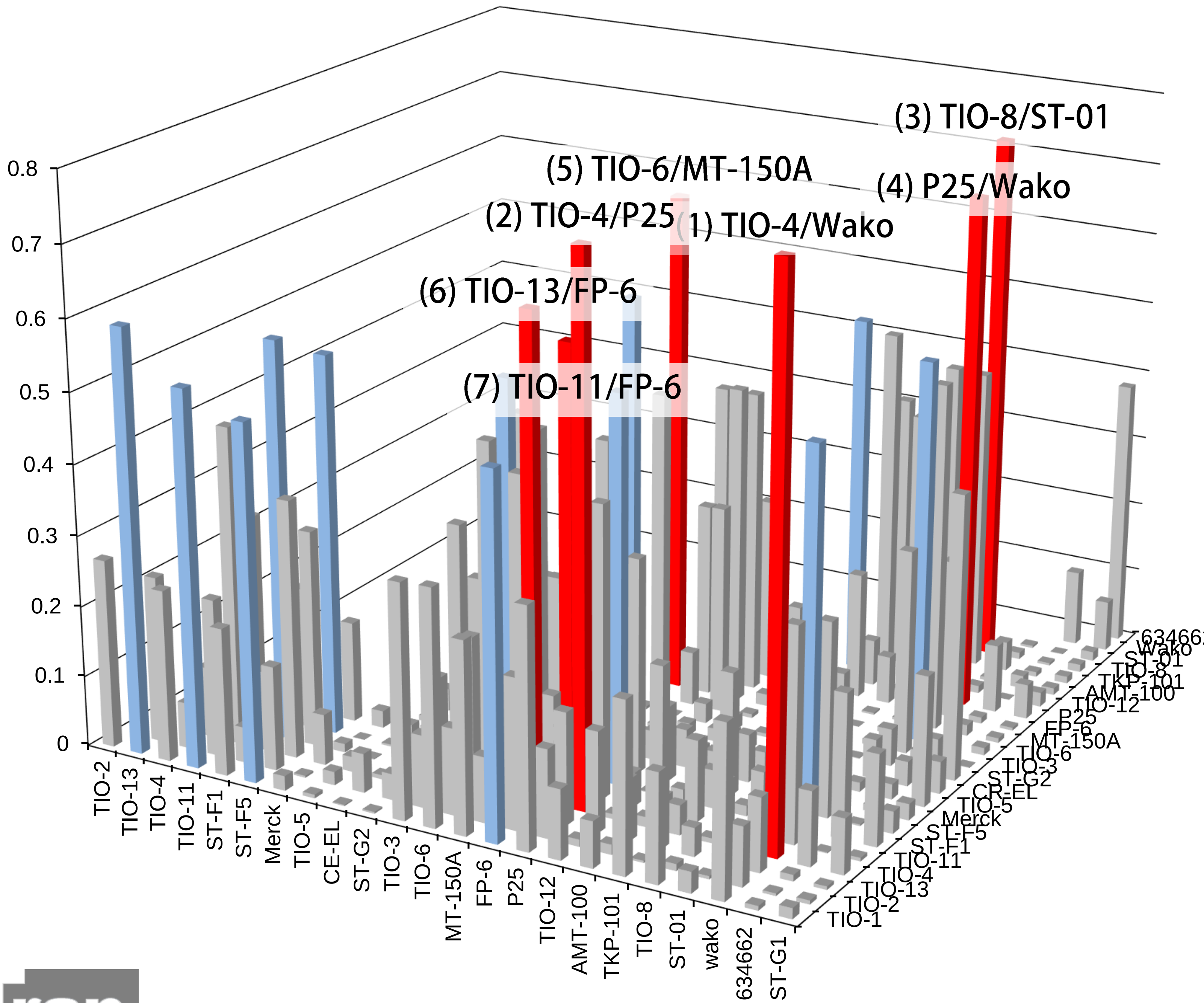

1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
second
third
another
first
second
third

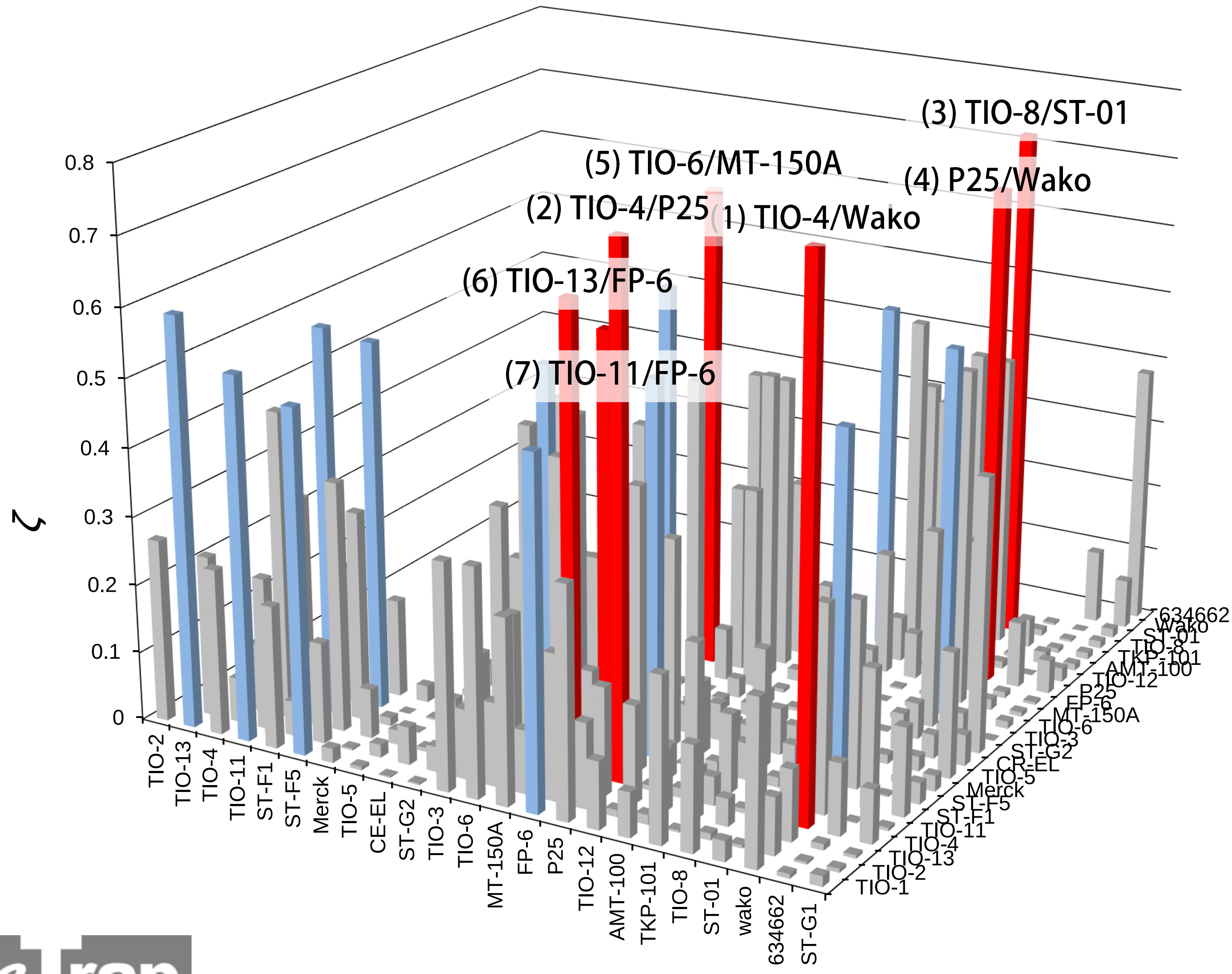


energy from VB top/eV
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
CB
<151>
FP-6
first
<163>
FP-6
second
<155>
FP-6
third
<173>
FP-6
0 10 20
ET density/mmol g-1



ζ
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
second
third
another
first
second
third


(3) TIO-8/ST-01
(5) TIO-6/MT-150A
(4) P25/Wako
(2) TIO-4/P25
(1) TIO-4/Wako
(6) TIO-13/FP-6
(7) TIO-11/FP-6
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
TIO-2
TIO-13
TIO-4
TIO-11
ST-F1
ST-F5
Merck
TIO-5
CE-EL
ST-G2
TIO-3
TIO-6
MT-150A
FP-6
P25
TIO-12
AMT-100
TKP-101
TIO-8
ST-01
wako
634662
ST-G1
634662
Wako
ST-01
TIO-8
TKP-101
AMT-100
TIO-12
P25
FP-6
MT-150A
TIO-6
TIO-3
ST-G2
CE-EL
TIO-5
Merck
ST-F5
ST-F1
TIO-11
TIO-4
TIO-13
TIO-2
TIO-1



(3) TIO-8/ST-01
(5) TIO-6/MT-150A
(4) P25/Wako
(2) TIO-4/P25
(1) TIO-4/Wako
(6) TIO-13/FP-6
(7) TIO-11/FP-6
ζ
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
TIO-2
TIO-13
TIO-4
TIO-11
ST-F1
ST-F5
Merck
TIO-5
CE-EL
ST-G2
TIO-3
TIO-6
MT-150A
FP-6
P25
TIO-12
AMT-100
TKP-101
TIO-8
ST-01
wako
634662
ST-G1
634662
Wako
ST-01
TIO-8
TKP-101
AMT-100
TIO-12
P25
FP-6
MT-150A
TIO-6
TIO-3
ST-G2
CR-EL
TIO-5
Merck
ST-F5
ST-F1
TIO-11
TIO-4
TIO-13
TIO-2
TIO-1

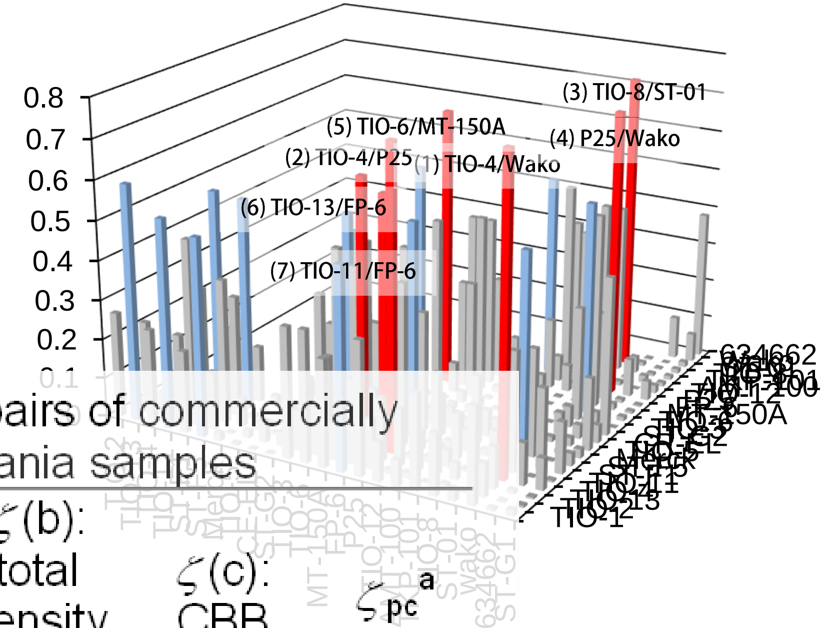
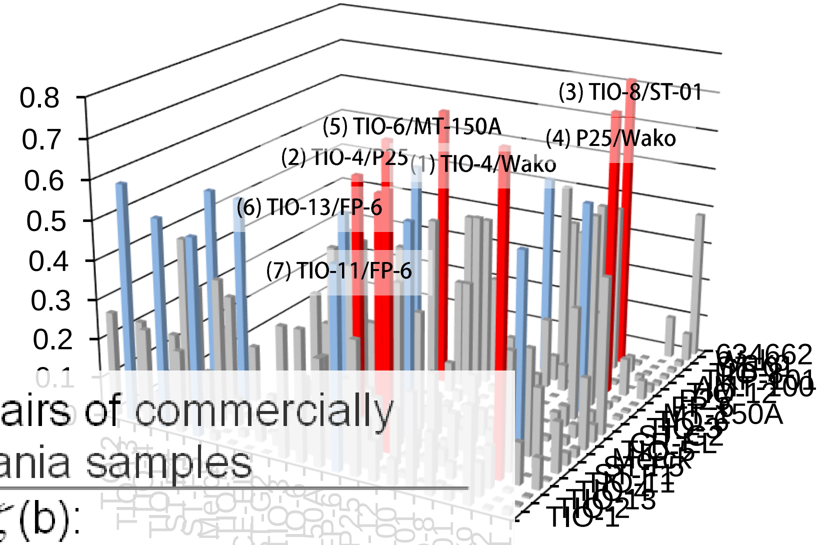


Table Top seven ranked high-ζ (> 0.6) pairs of commercially available or non-profitably provided titania samples

rank	pair		ζ	ζ(a): ERDT pattern shape	ζ(b): total density of ETs	ζ(c): CBB	ζ_{pc} [a]
1	TIO-4[b]	Wako[c]	0.788	0.863	0.941	0.970	0.901
2	TIO-4[b]	P25	0.760	0.810	0.939	0.999	0.884
3	TIO-8[b]	ST-01	0.751	0.851	0.885	0.996	0.839
4	P25	Wako	0.723	0.844	0.884	0.969	0.848
5	TIO-6[b]	MT-150A	0.705	0.856	0.828	0.995	0.793
6	TIO-13[b]	FP-6	0.684	0.847	0.827	0.976	0.748
7	TIO-11[b]	FP-6	0.615	0.620	0.998	0.994	0.697

[a]Average of ζ_{pc} for the three photocatalytic reactions. [b]Reference titania provided by Catalysis Society of Japan. [c]Code 207-11121 (208-18231), Wako Pure Chemical Industries Ltd.



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3	TIO-8[b]	ST-01	0.751	0.851	0.885	0.996	0.839
4	P25	Wako	0.723	0.844	0.884	0.969	0.848
5	TIO-6[b]	MT-150A	0.705	0.856	0.828	0.995	0.793
6	TIO-13[b]	FP-6	0.684	0.847	0.827	0.976	0.748
7	TIO-11[b]	FP-6	0.615	0.620	0.998	0.994	0.697

[a]Average of ζ_{pc} for the three photocatalytic reactions. [b]Reference titania provided by Catalysis Society of Japan. [c]Code 207-11121 (208-18231), Wako Pure Chemical Industries Ltd.

identification of

powders (metal oxide particles **with band gap and ETs**)

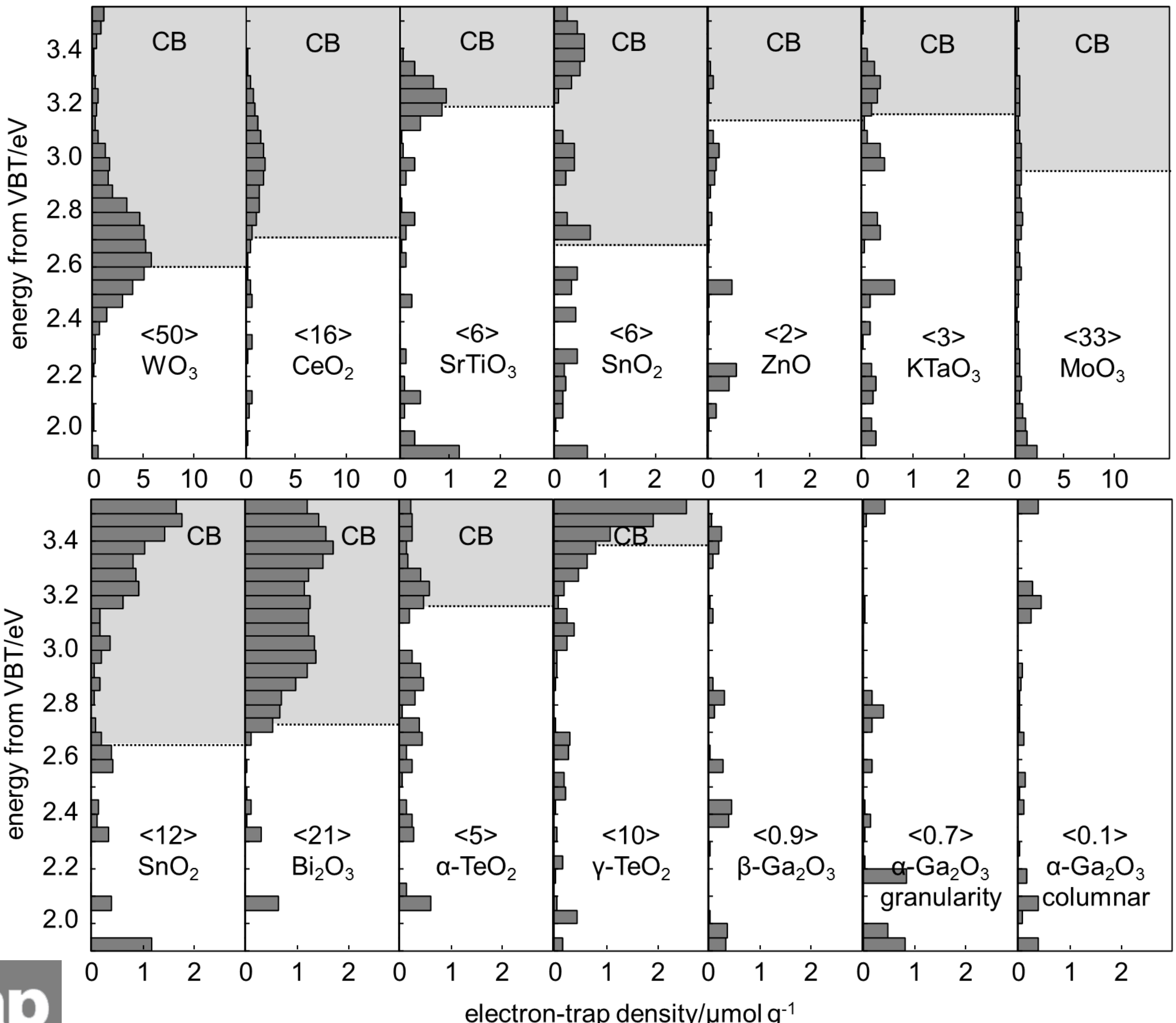
❖ bulk composition	XRD pattern
❖ bulk size (surface size)	nitrogen ads. (BET)
❖ surface structure	-----

identification of

powders (metal oxide particles with band gap and ETs)

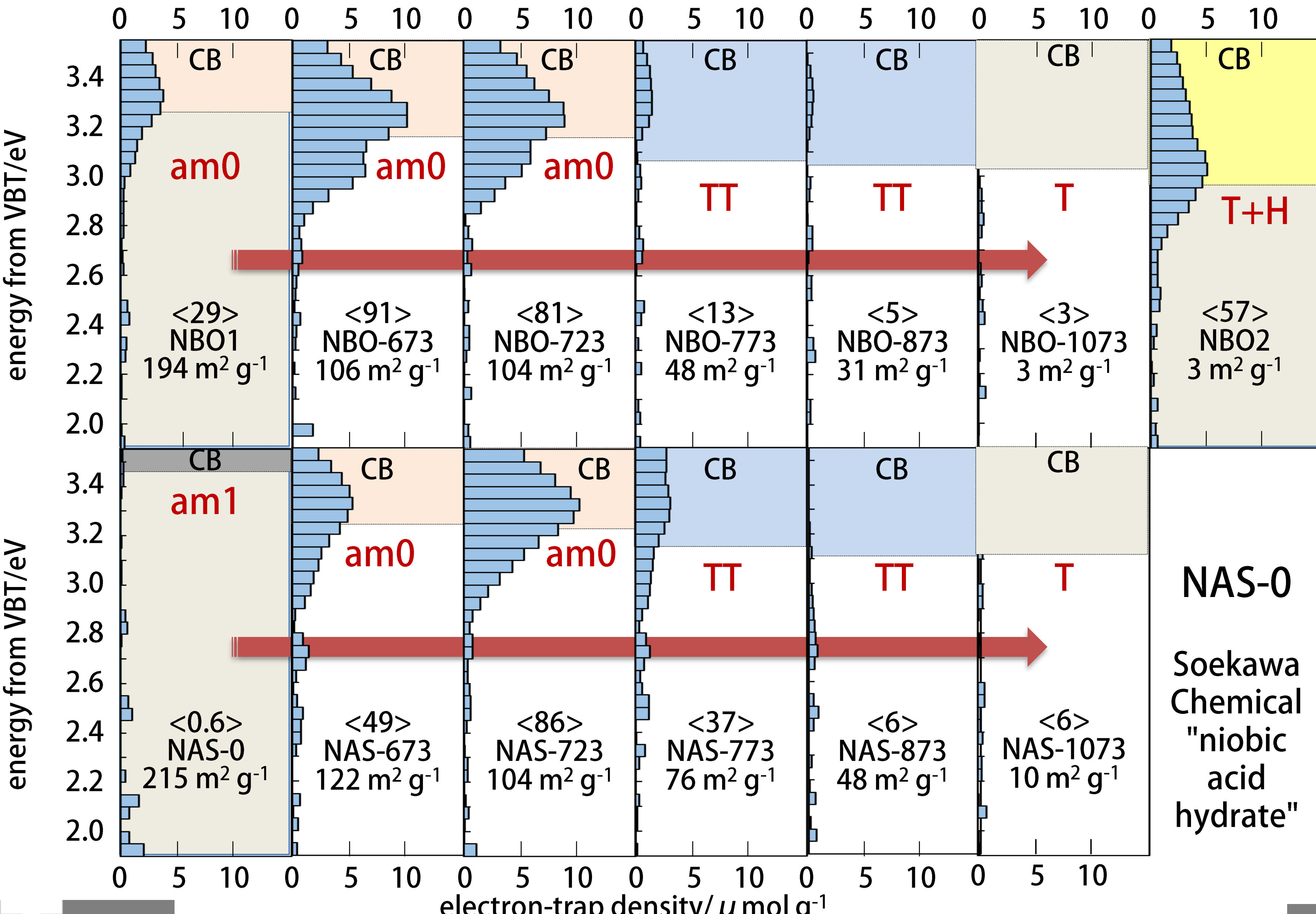
❖ bulk composition	CBB
❖ bulk size (surface size)	total ET density
❖ surface structure	ERDT pattern

ERDT and CBB for metal oxides other than titania



eTrap

niobia = niobium(V) oxide

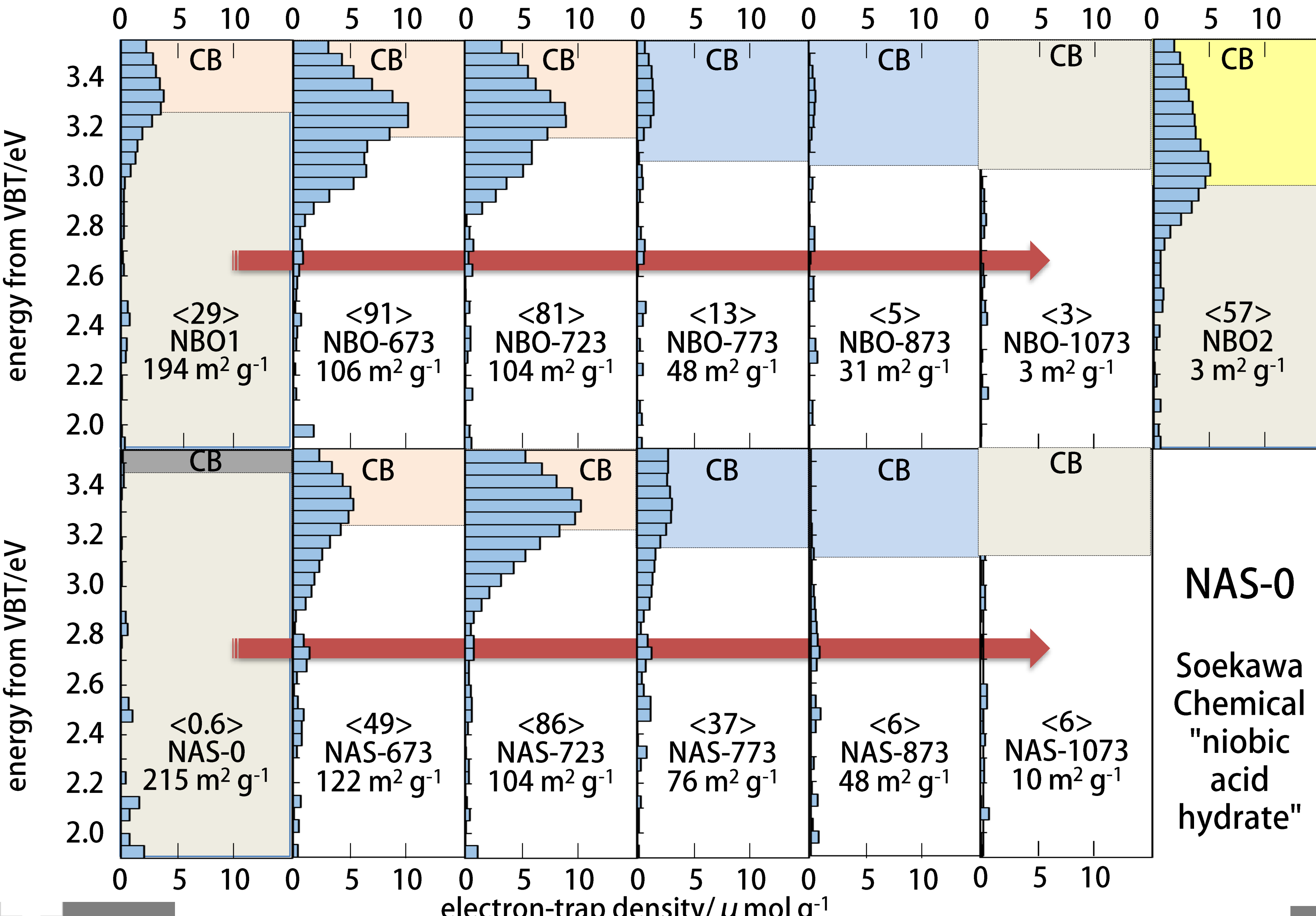


NAS-0

Soekawa Chemical "niobic acid hydrate"

e.Trap

niobia = niobium(V) oxide



X

e.g., titania particles

composition: TiO_2

crystalline form: anatase/rutile ...

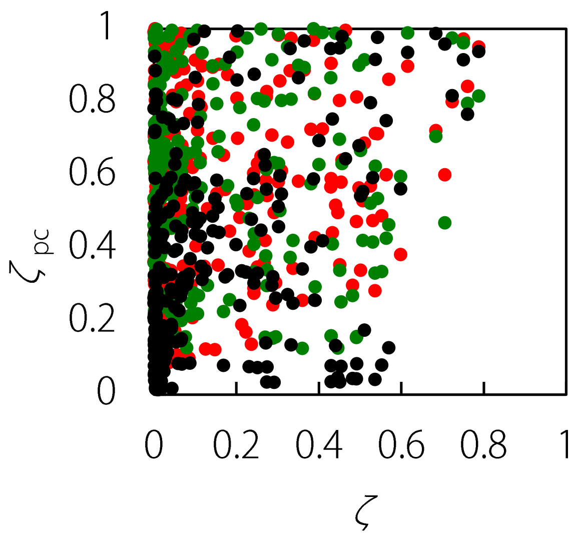
particle size

specific surface area

?

degree of coincidence

- $CH_3OH \rightarrow HCHO + H_2$
- $CH_3COOH + 2O_2 \rightarrow 2CO_2 + 2H_2O$
- $4Ag^+ + 2H_2O \rightarrow 4Ag + O_2 + 4H^+$



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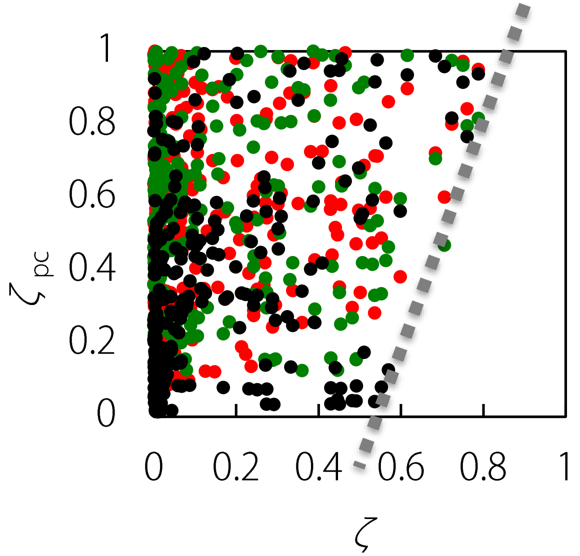

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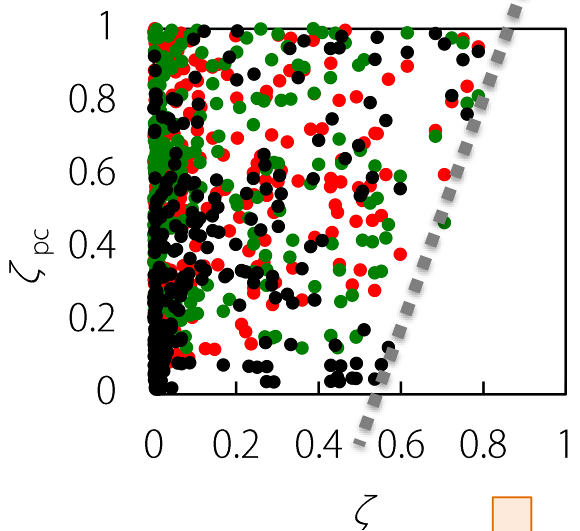
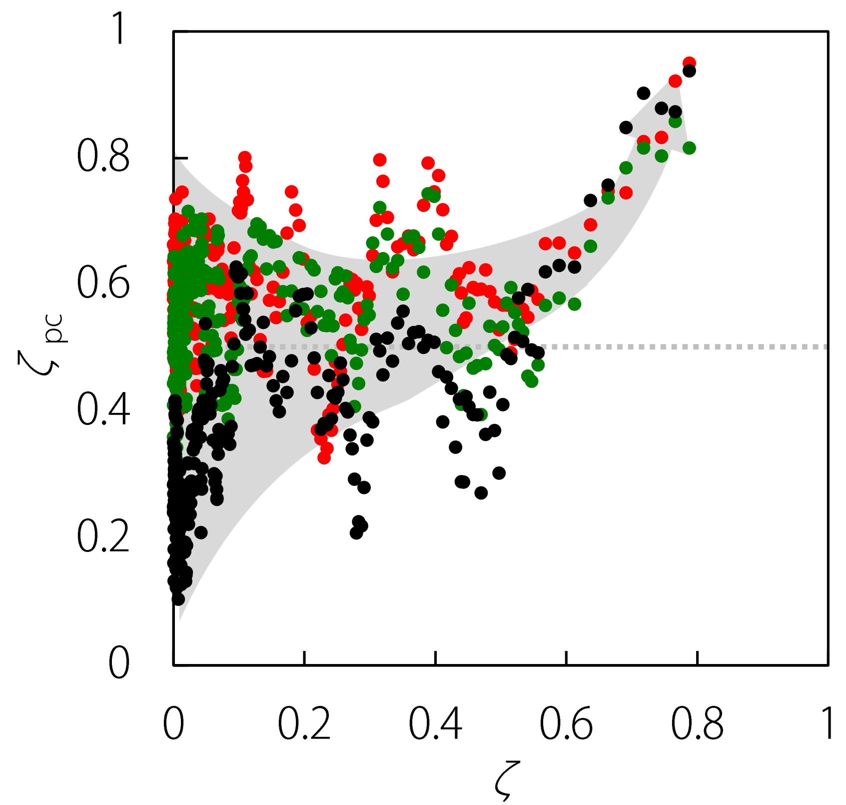


replotting of data with seven-point non-weighted moving average



ERDT/CBB pattern = decisive factor for photocatalytic activity

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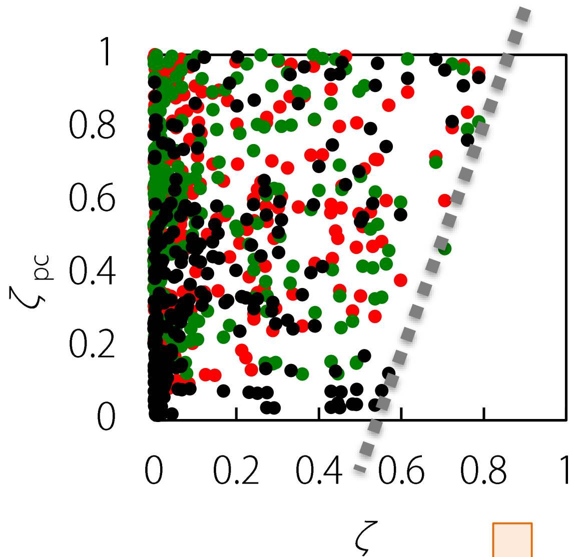

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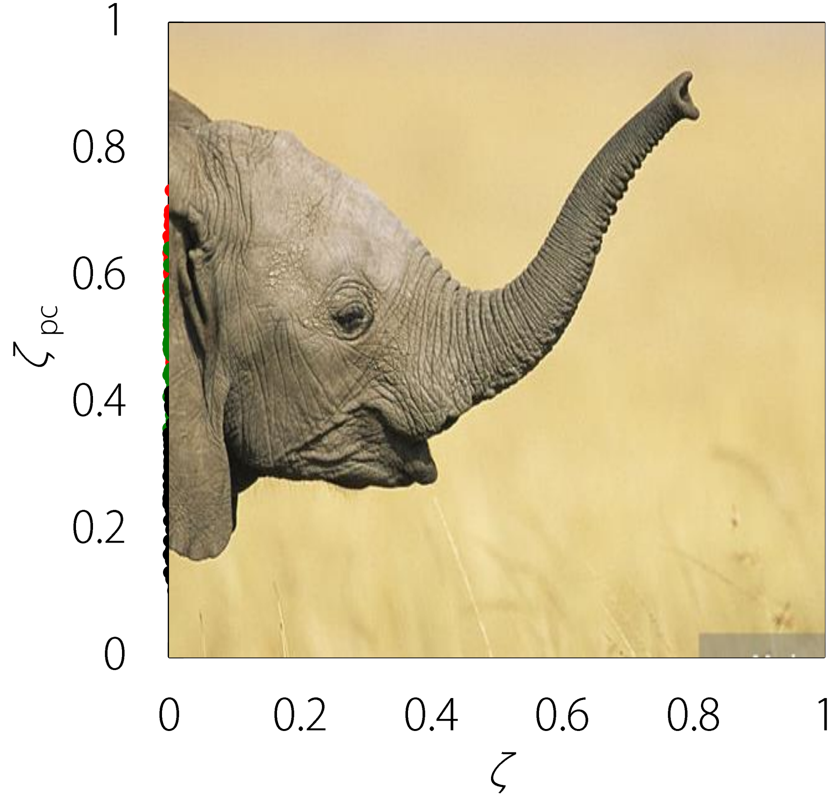


ERDT/CBB pattern = decisive factor for photocatalytic activity

H_2

$$CH_3OH \rightarrow HCHO + H_2$$

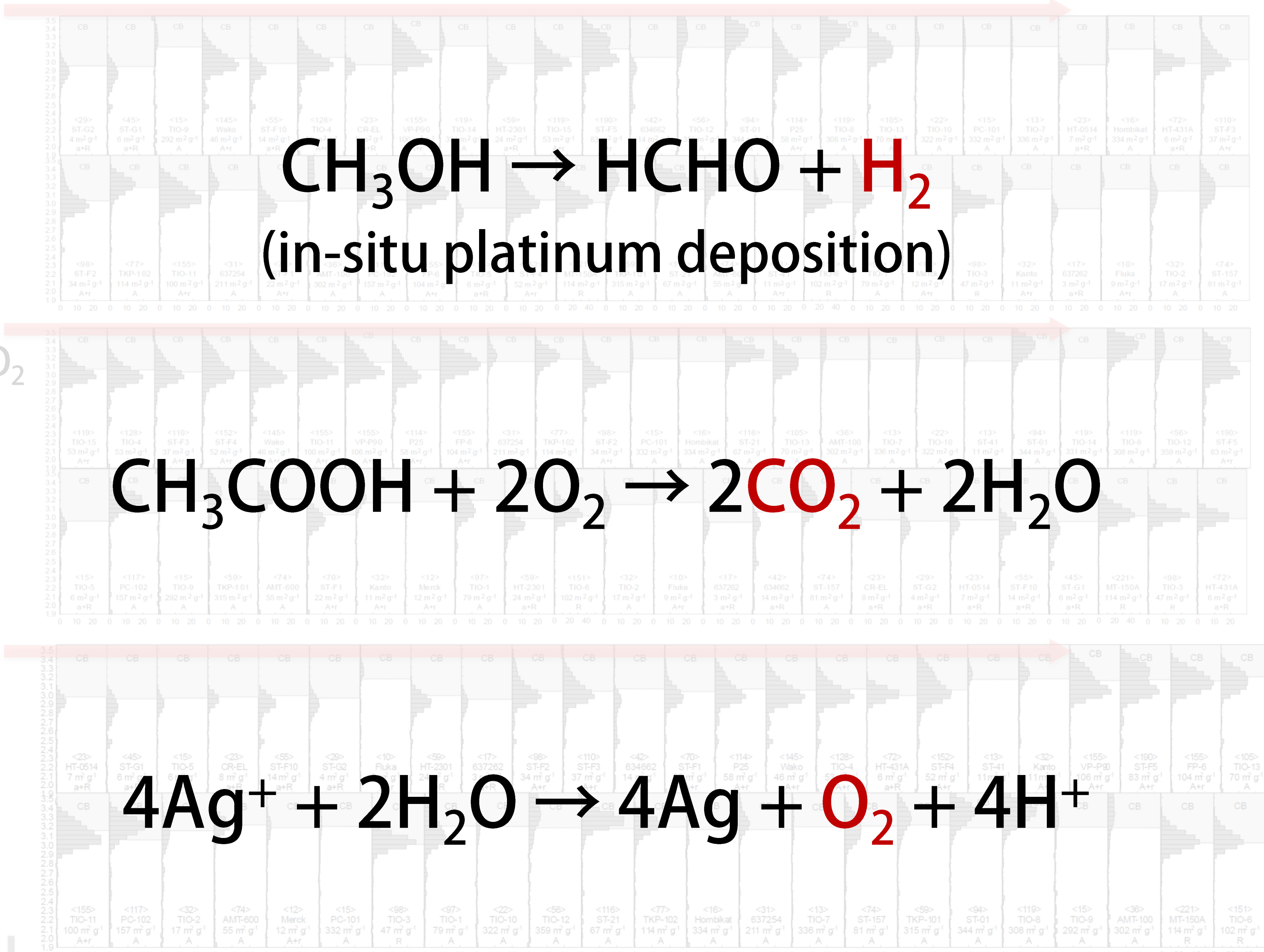
(in-situ platinum deposition)

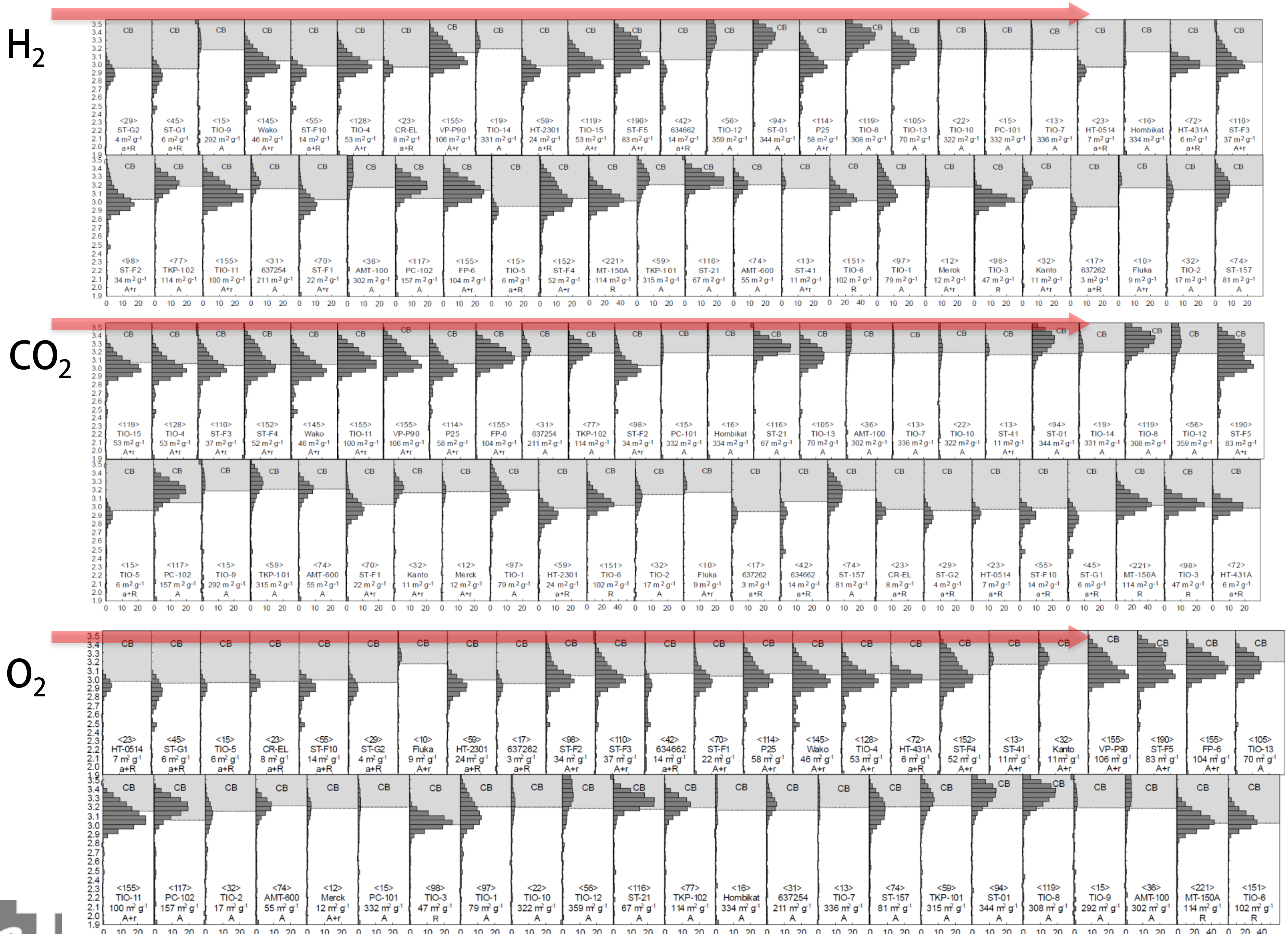
CO_2

$$CH_3COOH + 2O_2 \rightarrow 2CO_2 + 2H_2O$$

O_2

$$4Ag^+ + 2H_2O \rightarrow 4Ag + O_2 + 4H^+$$





H_2
CO_2
O_2

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A fingerprint of metal-oxide powders: energy-resolved distribution of electron traps

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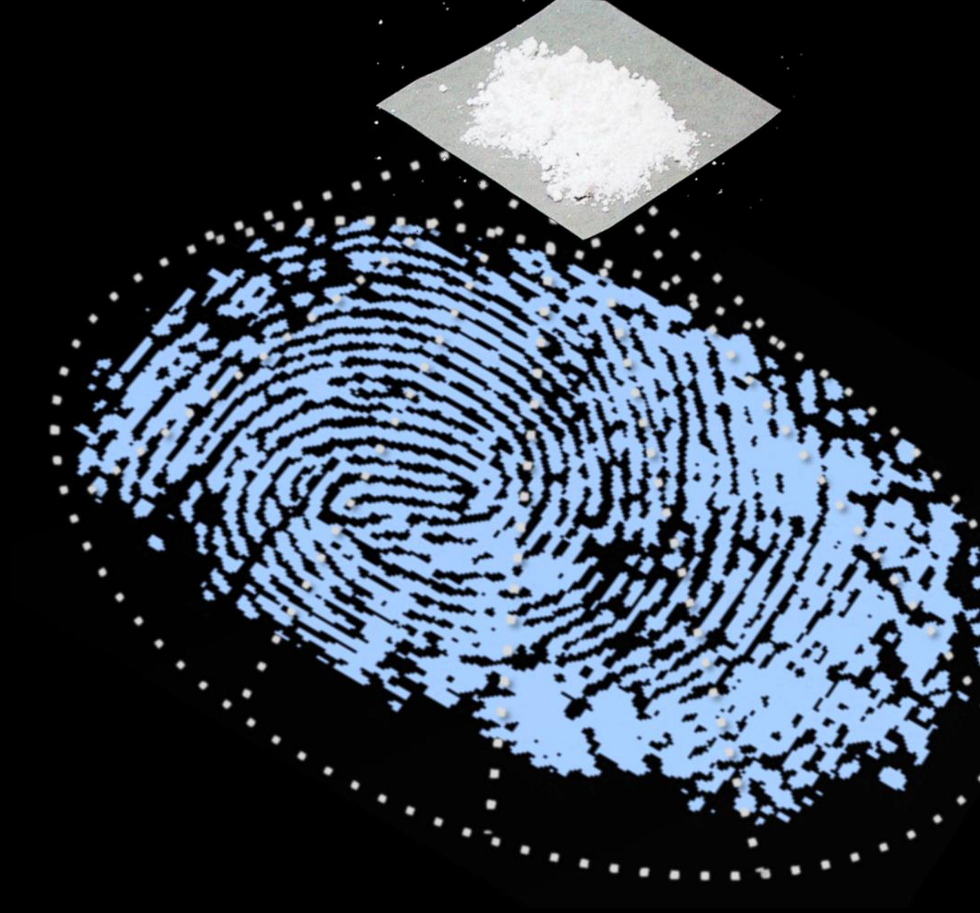
A fingerprint of metal oxide powders: Characterization and identification with energy-resolved distribution of electron traps



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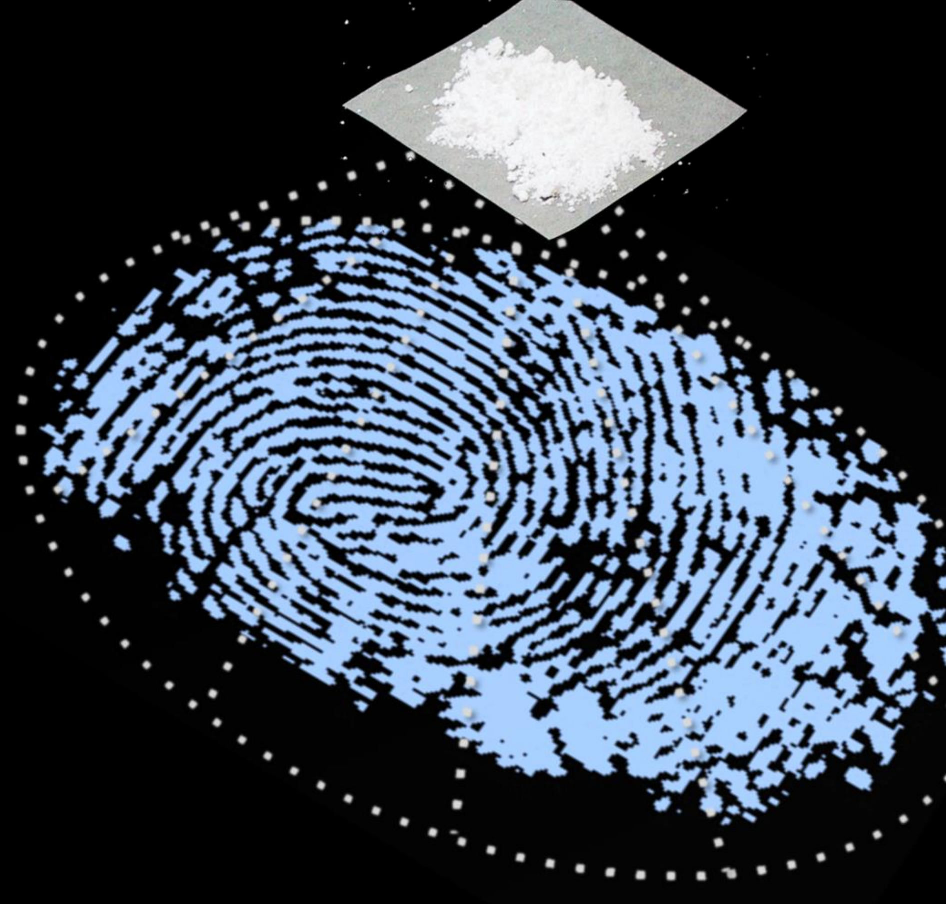

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organic compounds

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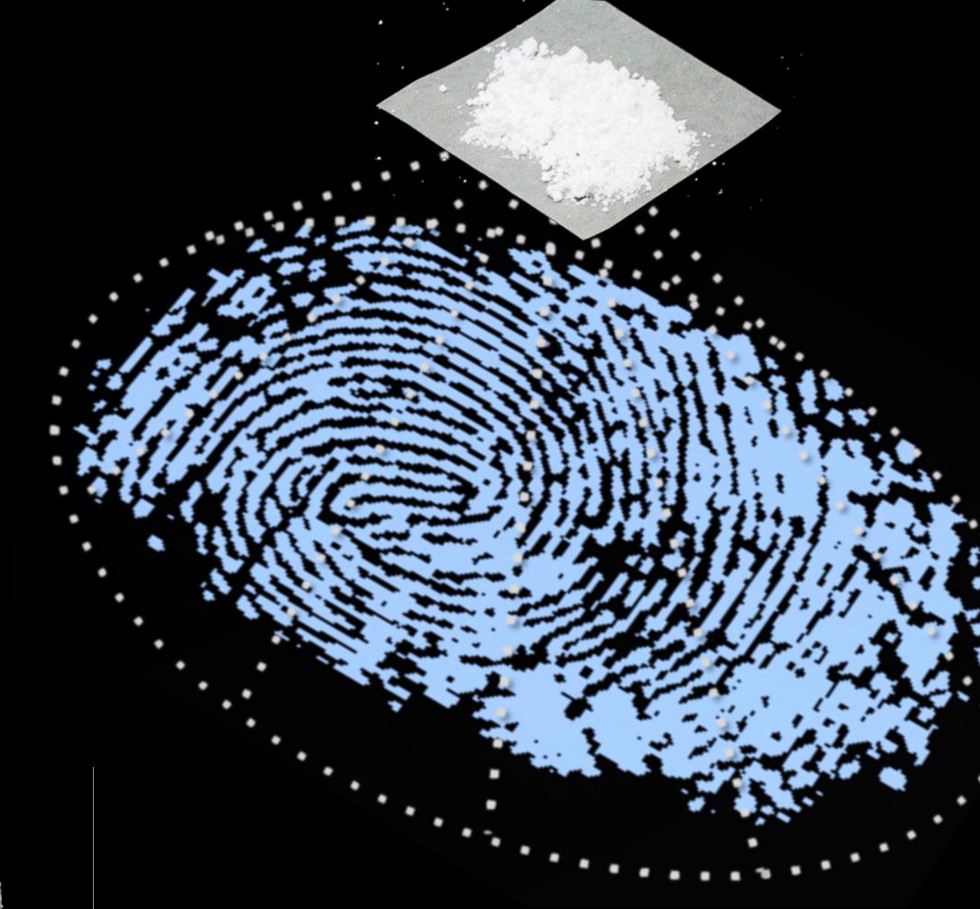

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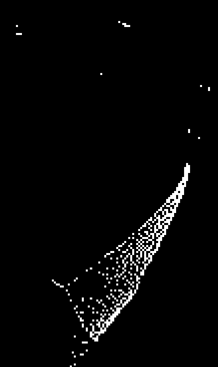
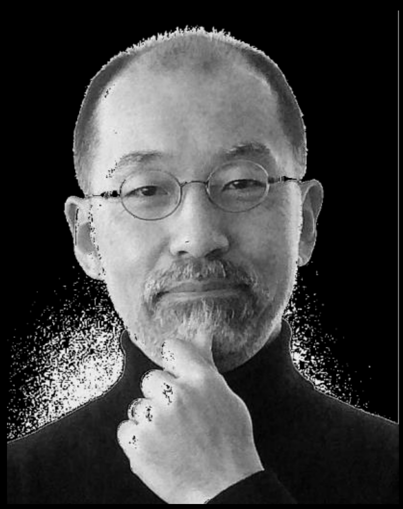


organic compounds



metal-oxide powders