

<学会発表>

NO.	発表者名	発表標題	学会名	開催地	発表年月
1	Mori, H.; Hirayama, N.; Komeiji, Y.; <u>Mochizuki, Y.</u>	Ab initio fragment molecular orbital-molecular dynamics (FMO-MD) study of solvation differences between cis- and trans-platins in water	ISTCP-7	Tokyo	2012.9
2	<u>Mochizuki, Y.</u>	Fragment molecular orbital calculations with ABINIT-MP(X)	ISTCP-7	Tokyo	2012.9
3	<u>入江 正浩</u>	分子結晶のフォトメカニカル機能 (招待講演)	レーザー学会 学術講演会 第32回年次大会	仙台	2012.1
4	<u>Edamoto, K.</u>	The electronic properties of transition metal phosphide surfaces: Angle-resolved and resonant photoemission studies	Progress in Applied Surface, Interface, and Thin Film Science III	Florence, Italy	2012.5
5	Itoh, S.; Katayama, M.; Sasagawa, K.; Yoshimura, N.; Sato, M.; <u>Yamatoka, H.</u>	Combined Experimental-Computational Study on the Reaction Pathway of $\alpha$ -Haloacetophenones with Nucleophiles: Possible Path Bifurcation in Addition/Substitution Mechanism	13th European Symposium on Organic Reactivity	Tallin, Estonia.	2011.9
6	<u>入江 正浩</u>	ジアリールエテン単結晶の フォトメカニカル機能 (招待講演)	特定領域研究 「フォトクロミズム の攻究と メカニカル 機能の創出」	東京	2011.11
7	<u>入江 正浩</u>	光機能を創る (特別講演)	大阪市工研シン ポジウム 2011	大阪	2011.11
8	<u>入江 正浩</u>	光に応答する分子と結晶 (特別講演)	分子科学討論会	札幌	2011.9
9	<u>Kuroda, C.</u> ; Hanai, R.; Tori, M.; Saito, Y.; Nagano, H.; Gong, X.	Furanoeremophilane as a new material for some <i>Ligularia</i> species in Yunnan and Sichuan	IUPAC 7 <sup>th</sup> International Symposium on Novel Materials and Synthesis (NMS-V)	上海	2011.10
10	<u>Morimoto, M.</u> ; <u>Irie, M.</u>	Photochemical Control of Dielectric Properties of a Diarylethene Crystal Having Hydrogen-Bonding Networks	14th International Symposium on Novel Aromatic Compounds (ISNA-14)	Oregon, USA	2011.7

11	Yamamoto, Y.; Hasegawa, H.; <u>Yamataka, H.</u>	Dynamic path bifurcation in the Beckmann reaction: Support from kinetic analyses	20th International Conference on Physical Organic Chemistry	Busan, Korea	2010.8
12	Yamamoto, Y.; Hasegawa, H.; <u>Yamataka, H.</u>	Dynamic path bifurcation in the Beckmann reaction: Support from kinetic analyses	20th International Conference on Physical Organic Chemistry	Busan, Korea	2010.8
13	<u>Irie, M.</u>	Photochromism of Diarylethene Molecules and Crystals: Application to Molecular Machinery (Plenary)	International Symposium on Molecular Nanotechnology	Nara, Japan	2010.12
14	<u>Irie, M.</u>	Photochromic Diarylethene Crystals: Application to Molecular Machinery (Plenary)	Japan-French Joint Seminar on Photochromism	Yokohama, Japan	2010.10
15	<u>Irie, M.</u>	Photochromic Diarylethene Crystals: Application to Molecular Machinery (Plenary)	Ciamician-Paterno Heritage Meeting	Ferrara, Italy	2010.7
16	<u>Morimoto, M.</u> ; <u>Irie, M.</u>	Photomechanical Effect of Diarylethene Co-crystals	6th International Symposium on Organic Photochromism (ISOP2010)	横浜	2010.10
17	Itoh, S.; Katori, T.; Akimoto, R.; Sato, M.; <u>Yamataka, H.</u>	Dynamic reaction pathways for the Schmidt reaction of benzylic ketones	12th International symposium on Physical Organic Chemistry	Fukuoka, Japan	2009.12
18	<u>Yamataka, H.</u> ; Sato, M.; Hasegawa, H.; Ammal, S. C	Dynamic Path Bifurcation for the Beckmann Reaction: Observation and Implication	Faraday Discussion 145	Cardiff, Great Britain	2009.9
19	<u>Mochizuki, Y.</u>	Large-scale correlated calculations with fragment molecular orbital scheme	CESTC, 2009	Dobogók, Hungary	2009.9
20	<u>Kuroda, C.</u> ; Hanai, R.; Nagano, H.; Tori, M.; Ohsaka, A.; Hirota, H.; Gong, X.	Difference in chemical composition of some <i>Ligularia</i> species between Yunnan and Sichuan	IUPAC 5 <sup>th</sup> International Symposium on Novel Materials and Synthesis (NMS-V)	上海	2009.10

21	<u>Kuroda, C.;</u> <u>Hanai, R.;</u> <u>Torihata, A.;</u> <u>Tori, M.;</u> <u>Nagano, H.;</u> <u>Gong, X.</u>	Ecological chemistry of furanoeremophilanes in <i>Ligularia</i>	9 <sup>th</sup> International Meeting of Biosynthesis and Function of Isoprenoids in Plants	東京	2009.5
22	<u>Morimoto, M.</u>	Crystal structures and photochromic performance of diarylethene single crystals	Second Japanese- French Workshop on NanoBioPhoto- Nics	Marseille, France	2009.10
23	<u>Mochizuki, Y.</u>	Recent Progress in the Fragment Molecular Orbital Method	CECAM	Lyon, France	2008.5
24	<u>Irie, M.</u>	Photochromism of Diarylethene Single Crystals – Reversible Color and Shape Changes on Photoirradiation (Plenary)	New Horizons of Photochromism: From Desing of Molecules to Applications (JSPS-CNRS Seminar)	Arras, France	2008.10
25	<u>Irie, M.</u>	Photochromism of Diarylethenes (Award Lecture)	Theodor-Förster -Preis Lecture 2008	Biefeld, Germany	2008.10
26	<u>Irie, M.</u>	Photochromism of Diarylethene Single Crystals – Reversible Color and Shape Changes on Photoirradiation (Keynote)	IUCr 2008	Osaka, Japan	2008.8
27	<u>Irie, M.</u>	Photochromic Diarylethene Molecules and Crystals (Plenary)	IUPAC Symposium on Photochemistry	Göthen- burg, Sweden	2008.7
28	<u>Irie, M.</u>	Photochromism of Diarylethene Single Crystals (Invited)	Organic Chemistry for Functional Materials	Uppsala, Sweden	2008.4