ワークショップ
「複雑物質系の分子理論の発展」
名古屋大学東山キャンパス ES総合館・ESホール
令和６年３月１４日

“複雑物質系の分子反応理論を目指して”
“Toward the Theory of Molecular Reactions in Complex Material Systems”

長岡正隆
Masataka Nagaoka
名古屋大学 情報学部/大学院情報学研究科
自然情報学科　複雑システム系/複雑系科学専攻
（名大情報文化学部/大学院人間情報学研究科
平成10年7月採用）

Ncube Nagaoka Laboratory

Outline

JOURNEY “DEPARTURE”

For copyright reasons, the images are not displayed.

Ncube Nagaoka Laboratory

Outline

§1 At the Beginning
§2 Toward ”Fukui’s Lab”!
~From physics to chemistry!~
§3 Go on ! “Nobel Prize” !
§4 Nagaoka Lab Starts ! A Departure ! ?
What we have done before leads to what we have started “newly”!
~A private version of ‘recent chemistry’~
§5 Evolving! Toward the Complexity
§6 Concluding Remarks
~Are we carrying on the spirit of Fukui’s lab?~
§7 Acknowledgments

JOURNEY “DEPARTURE”

For copyright reasons, the images are not displayed.

Ncube Nagaoka Laboratory

:01

§1 At the Beginning

Asahi Weekly DIGITAL

No “Blueprints” Left Behind, but Connecting “Hearts and Minds”: The night high school students burn the giant dragon they spent six months building”

Daisuke Shimizu 2023, Jul. 1st 08:00

“Students spend more than half a year creating **a huge dragon object** and erect it on the ground for the festival. They **dismantle** it and **burn** it at an evening festival. …

This is a traditional event that has been handed down for nearly half a century at Nagano Prefectural **Suzaka High School** in Suzaka City. The school's emblem is the Miyama Gentian, (Rindo in Japanese), and there is a nearby mountain called **Garyu-zan**, so the students create objects at the "**Rindo Festival**" (cultural festival) using the **dragon** as a symbol. This tradition began in 1967.

Half a century ago, a physics teacher said

It has a thick timber skeleton, and in some years it exceeds 10 meters in height. However, the blueprints have not been handed down to the next generation, and the words of a **physics teacher**, a licensed architect, who played a central role in designing the framework 50 years ago, are still spoken today: "Don't leave the blueprints, burn them”. The leader of this year's dragon production: ”That's the interesting part and the good part. It is not the paper (blueprints) but the feelings that connect us.”

NHK Documentary Series Ningen Document

*For copyright reasons, the images are not displayed.

“Make a Dragon Thrust into the Sky: Nagano Suzaka High School Cultural Festival”
(2006.9.8)

Brief Personal History

era	BC	
77(S52)03	22	Grad. Suzaka High Schl
82(S57)03	16	Grad. Fac. Eng. KU.
84(S59)03	14	Completed MC, KU.
87(S62)03	11	Completed DC, KU.
88(S63)04	10	JSPS*Fellow (IFC)
91(H03)04	07	Deputy Chief RO (IFC)
93(H05)06	05	**US-Belgium Summer Tour**
97(H09)09	01	Chief RO (IFC)
98(H10)01	00	Leaving (Prof. Fukui Passed away)

Prof. Fukui awarded N!

*JSPS: Japan Society for the Promotion of Science

98(H10)07	Change to NU Assoc. Prof. of GS. of Human Informatics, NU
10	JST*Computational Science and Technology Specific Research and Development Promotion Project: **ACT-JST** ”Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems”
*JST: Japan Science and Tech Corporation	
Birth of Lab Ncube !	Birth of ”Three “Non”s” !!
02(H14)03	Conference CRN³ (Clarifying Non-equilibrium non-stationarity characteristic of chemical reaction phenomena) (Grant-in-aid: C)
02(H14)09	Prof. (Human Info)
03(H15)04	Prof. (Info. Sci.)
04(H16)04	21st Century COE "Computational Science Frontiers"

06(H18)10	JST*Core Research for Evolutionary Science and Technology: **CREST** "Research Development of Multiscale Simulation of Aggregation Reaction Systems“
07(H19)04	Minor ailment
08(H20)12	**”Ready-to-Use Manual for Molecular Simulation Beginners”** Published !
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13(H25)10	JST*Core Research for Evolutionary Science and Technology: **CREST** “Establishment of Computational Molecular Tech-nology towards Macroscopic Chemical Phenomena”
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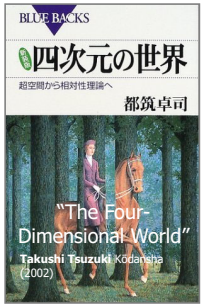
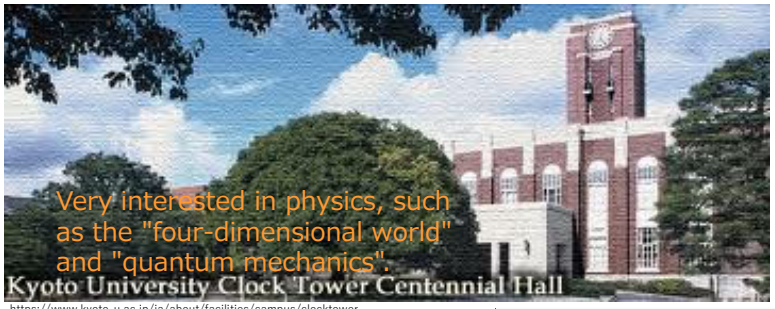
15(H27)12	PACIFICHEM2015
16(H28)04	MSCRS2016 (JSPS Japan-Brazil+NU)
17(H29)04	Prof. (Fac. and GS. of Informatics)
18(H30)09	Kanreki (60th BD)
20(R02)12	PACIFICHEM2020
23(R05)03	StudyCamp2022

§2 Toward "Fukui's Lab"! From Physics to Chemistry!

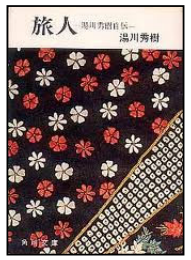
Entered Kyoto University (1978)





https://www.kyoto-u.ac.jp/ja/about/facilities/campus/clocktower

Hideki Yukawa: First Japanese to win the Nobel Prize in Physics (1949).



"**Traveler: The Autobiography of Hideki Yukawa**" (Kadokawa paperback,1960)

CLOSE ENCOUNTERS OF THE THIRD KIND
We are not alone.

STAR WARS
Episode 4/A New Hope

Galaxy Express 999

For copyright reasons, the images are not displayed.

Entered Kyoto University (1978, BC21)

B1

Evening News 1978.7.27

Birth of Test Tube Baby (July, UK)

https://www.kyoto-u.ac.jp/ja/about/facilities/campus/clocktower

"**Candies**" disbanded (April, Korakuen)(Back to being normal girls!)

NHK 2023 morning drama "Boogie Woogie" starts on Oct. 2nd, featuring heroine **Ms. Shuri**, a child of **Ms. Ran Itoh**, a member of "Candies".

STAR WARS
Episode 4/A New Hope

Galaxy Express 999

For copyright reasons, the images are not displayed.

Entered Kyoto University (1978, BC21)

B1

Evening News 1978.7.27

Birth of Test Tube Baby (July, UK)

https://www.kyoto-u.ac.jp/ja/about/facilities/campus/clocktower

"**Candies**" disbanded (April, Korakuen)(Back to being normal girls!)

http://c5557.a.la9.jp/kyotosiden-1978-3.htm

In front of Club House of "Kyoto University Symphony Orchestra" (north of Higashiyama-Konoe intersection)
(The club house was destroyed by fire on Oct. 31, 1996)

STAR WARS
Episode 4/A New Hope

Galaxy Express 999

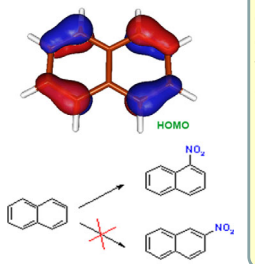
All Kyoto tram lines were discontinued in the September!

For copyright reasons, the images are not displayed.

The 1981 Nobel Prize in Chemistry
Awarded to Prof. Fukui! (1981, BC17) B4

https://www.kyoto-u.ac.jp/contentarea/ja/issue/kurenai/documents/25.pdf

シリーズ映画第5作(1967)



https://people.chem.ucsb.edu/kahn/kalju/chem109C/FMO_Theory.html

"It's October 19, 1981, 9:50 p.m. The phone rings. **My husband casually stands and picks up the telephone in the hallway, while my daughter and I are glued to Sean Connery's "007," which is in its climax.** ... I look over at him and see a slightly reddish expression, an angry look in his eyes, and a rare blood vessel on his neck. ··· **While I was wondering what was going on, I was distracted by the action of "007,"** when suddenly the following words appeared on the TV screen in the form of a news bulletin: **"Professor Kenichi Fukui of Kyoto University won the Nobel Prize.""**

(text by Prof. Fukui's wife)

Hooray for Prof. Fukui! (811020) B4

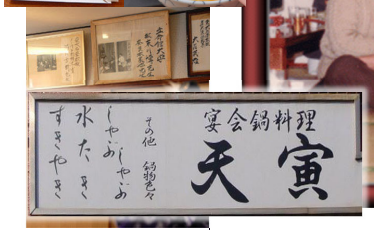
https://flyteam.jp/photo/854929

ANN NEWS

"Nobel Prize in the Shōwa Era – Japan's First Nobel Prize in Chemistry: Kenichi Fukui"

For copyright reasons, some images are shown in low resolution or are not displayed.

Fukui Lab's Year-End Party 1981 (811226) B4



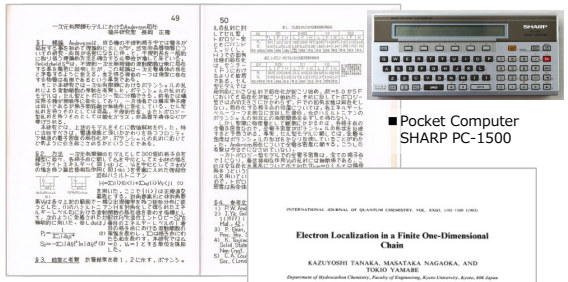
Tastes loved by Nobel Prize-winning professors

At the 1981, Year-End Party (in "Ten-Tora" (a Japanese pub (Izaka-ya)) (Moto-Tanaka, Kyoto)) Sat., Dec. 26, 1981

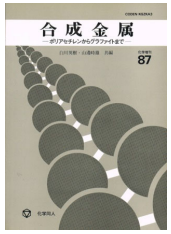
A Last Student of Prof. Fukui ('82 Spring) B4

Bachelor's Thesis: "Anderson Localization in One-dimensional Finite Chain Models"

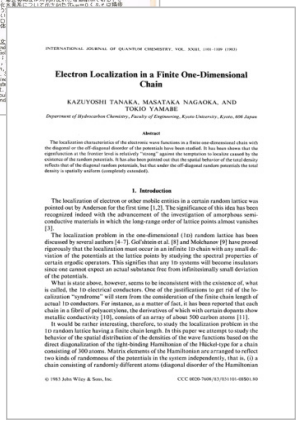
After the presentation of graduation theses at the entrance of building of Department of Hydrocarbon Chemistry (Taken on Mar. 11, 1982)



■Pocket Computer SHARP PC-1500



"Synthetic Metals" (Kagaku Dojin)



A Last Student of Prof. Fukui ('82 Spring) B4

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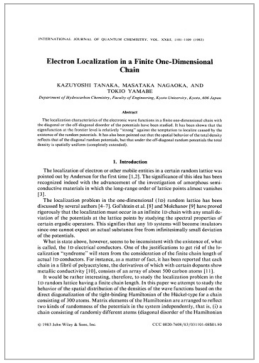

Electron Localization in a Finite One-Dimensional Chain

KAZUYOSHI TANAKA, MASATAKA NAGAOKA, AND TOKIO YAMABE

Department of Hydrocarbon Chemistry, Faculty of Engineering, Kyoto University, Kyoto, 606 Japan

■The total electron density does not change in non-diagonal disorder! !

$$\pi_{r,st}\left(\equiv\frac{\partial q_r}{\partial\beta_{st}}\right)=0$$

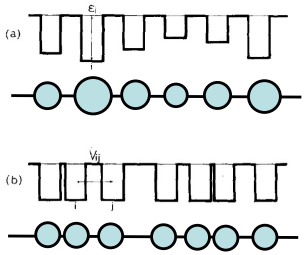

Fig. 1. Potential and one-dimensional chain diagram (a) diagonal disorder and (c) off-diagonal disorder

$$q_r=2\sum_{j=1}^{occ}c_{rj}^2$$

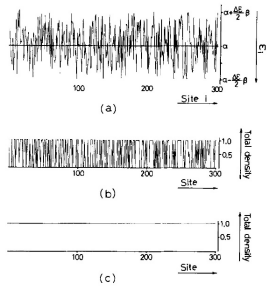

Fig 2. (a) Potential and total electron density ((b) diagonal disorder and (c) off-diagonal disorder)

C.A. Coulson
(1910-1974)
Oxford大('45-'47)
King's College London
('47-'??)

H.C. Longuet-Higgins
(1923-2004)
Cambridge大('54-'67)
Edinburgh大('67-'74)

■The atom-bond polarizability
(Coulson & Longuet-Higgins, 1947)

$$\pi_{r,st}=\frac{\partial q_r}{\partial\beta_{st}},\quad \pi_{st,r}=\frac{\partial p_{st}}{\partial\alpha_r},$$

・C.A. Coulson, H.C. Longuet-Higgins, *Proc. R. Soc. Londn*, **A192**, 16 (1947)

The Last Party (Farewell Party)! (820320) B4

The current "Tozanso" appears to have been newly built in 2008. Beg for information!

The Last Party (Farewell Party)! (820320) B4

The really last snapshot as Fukui lab!

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87(S62)03	11	Completed DC, KU. **ICSM'86**
88(S63)04	10	JSPS*Fellow (IFC)
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97(H09)09	01	Chief RO (IFC)
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Prof. Fukui awarded NP

98(H10)07	Assoc. Prof. of GS. of Human Informatics, NU (Change to NU)
10	JST*Computational Science and Technology Specific Research and Development Promotion Project: **ACT-JST** "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems"
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*JST: Japan Science and Tech Corporation

Birth of Lab Ncube !

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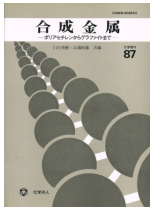
18(H30)09	Kanreki (60th BD)
20(R02)12	PACIFICHEM2020
23(R05)03	StudyCamp2022

ICSM’86（860601-06）

D3

～“1986 International Conference on Science and Technology of Synthetic Metals”～



Reception：
Holyday Inn Kyoto

Banquet：
Kyoto Hotel

ICSM’86（860601-06）

D3

Ultra Seven：
Episode 14
“Ultra Guard to the West (Part I)”
(1968)

Ultra Seven
Blu-ray

六甲防衛センター Rokko Center of Defense
(Terrestrial Defense Force (TDF)) Changed to
KICH (国立京都国際会館)

国立京都国際会館
KYOTO INTERNATIONAL CONFERENCE HALL

Ultra Seven
Episode 14 – *“Ultra Guard to the West (Part 1)”*
Battle scene between Ultra Seven and King Joe at the Rokko Defense Center

For copyright reasons, the images are not displayed.

ICSM’86（860601-06）

D3

Ultra Seven：
Episode 14
“Ultra Guard to the West (Part I)”
(1968)

Ultra Seven
Blu-ray

六甲防衛センター Rokko Center of Defense
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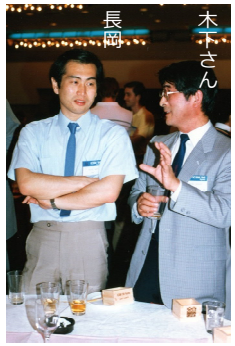
KICH (国立京都国際会館)

国立京都国際会館
KYOTO INTERNATIONAL CONFERENCE HALL

BCS Theory of Superconducting



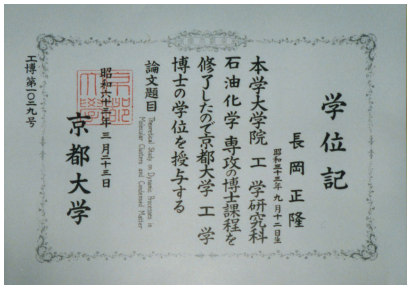
Sea Bathing (I-ne (伊根))(860828-30)

Whose bag?

Inn “Shibata”
(しばた荘)
Guest room

My Inception of Doc. Degree (Dr.Eng.)

Dr. Yasunori Nishijima, the 21st President of Kyoto University, hands him his doc. degree.



学位記

長岡正隆

昭和三十五年九月十二日生

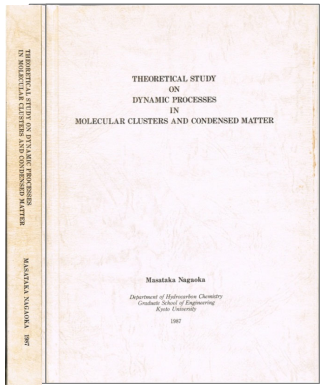
本学大学院工学研究科石油化学専攻の博士課程を修了したので京都大学工学博士の学位を授与する

論文題目 Theoretical Study on Dynamic Processes in Molecular Clusters and Condensed Matter

昭和六十三年三月二十三日

京都大学

工博第一〇二九号



THEORETICAL STUDY
ON
DYNAMIC PROCESSES
IN
MOLECULAR CLUSTERS AND CONDENSED MATTER

Masataka Nagaoka

Department of Hydrocarbon Chemistry
Graduate School of Engineering
Kyoto University

1987

Title: Theoretical Study on Dynamic Processes in Molecular Clusters and Condensed Matter

In March 1988, I completed my doctoral studies at the Graduate School of Engineering, KU, and was awarded a doctorate in engineering.

https://www.iaqms.org/deceased/hall.php

Prof. G.G. Hall (one of the sub-examiners)

Brief Personal History

era	BC	
77(S52)	03 22	Grad. Suzaka High Schl
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97(H09)	09 01	Chief RO (IFC)
98(H10)	01 00	Leaving (Prof. Fukui Passed away)

Prof. Fukui awarded NP

Institute for Fundamental Chemistry

Ncube Nagaoka Laboratory

Outline

JOURNEY "DEPARTURE"

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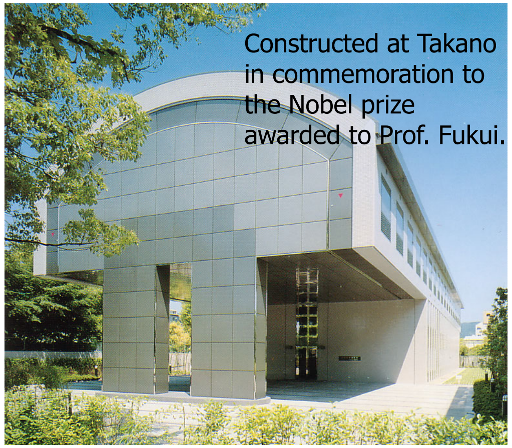
Ncube Nagaoka Laboratory

:01

§3 Go on ! "Nobel Prize" !

Institute for Fundamental Chemistry (880401)

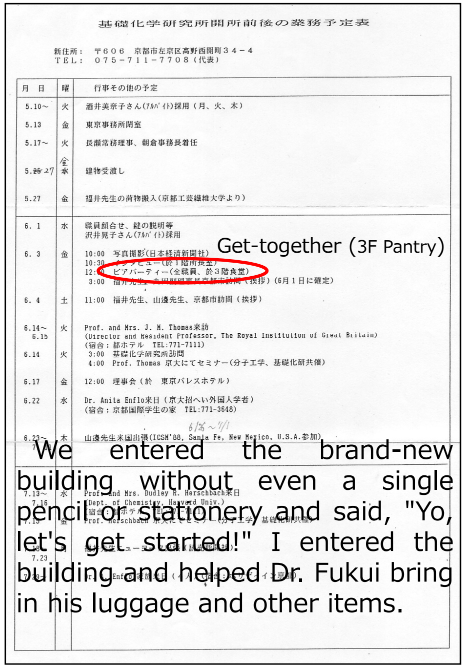
((Present) Fukui Institute for Fundamental Chemistry, Kyoto University)



https://www.iaqms.org/deceased/hall.php

On April 1st,1988, I moved to the Institute as a researcher to welcome Prof. Fukui who was supposed to be inaugurated as Director on June 1.

First Get-together (3F Pantry)(880601We)

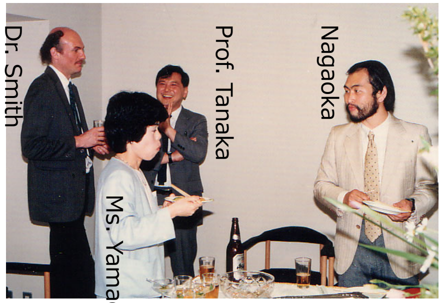


基礎化学研究所開所前後の業務予定表

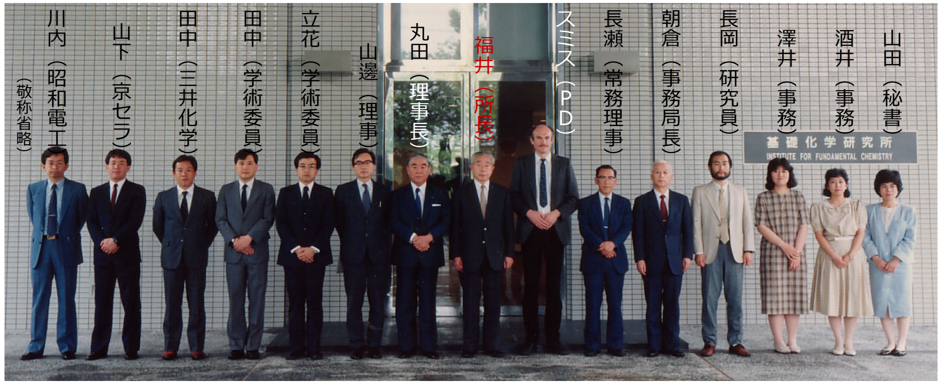
新住所：　〒606　京都市左京区高野西開町34－4
TEL：　075－711－7708（代表）

月　日	曜	行事その他の予定
5.10～	火	酒井美奈子さん(ｱﾙﾊﾞｲﾄ)採用（月、火、木）
5.13	金	東京事務所閉室
5.17～	火	長瀬常務理事、朝倉事務長着任
5.~~26~~ 27	金 ~~水~~	建物受渡し
5.27	金	福井先生の荷物搬入（京都工芸繊維大学より）
6. 1	水	職員顔合せ、鍵の説明等 沢井晃子さん(ｱﾙﾊﾞｲﾄ)採用
6. 3	金	10:00　写真撮影（日本経済新聞社） 10:30　インタビュー（於1階所長室） 12:00　ビアパーティー（全職員、於3階食堂） 3:00　福井先生、丸田副理事長京都市訪問（挨拶）（6月1日に確定）
6. 4	土	11:00　福井先生、山邊先生、京都市訪問（挨拶）
6.14～6.15	火	Prof. and Mrs. J. M. Thomas来訪 (Director and Resident Professor, The Royal Institution of Great Britain) （宿舎：都ホテル　TEL:771-7111）
6.14	火	3:00　基礎化学研究所訪問 4:00　Prof. Thomas 京大にてセミナー（分子工学、基礎化研共催）
6.17	金	12:00　理事会（於　東京パレスホテル）
6.22	水	Dr. Anita Enflo来日（京大招へい外国人学者） （宿舎：京都国際学生の家　TEL:771-3648）
6.23～	木	山邊先生米国出張(ICSM'88, Santa Fe, New Mexico, U.S.A.参加) 6/26～7/1
7.13～7.16	水	Prof. and Mrs. Dudley R. Herschbach来日 (Dept. of Chemistry, Harvard Univ.)

We entered the brand-new building without even a single pencil or stationery and said, "Yo, let's get started!" I entered the building and helped Dr. Fukui bring in his luggage and other items.



Commemorative Photo on the Opening Day of IFC (880601, We) (without honorifics)



On June 1, 1988, after a dinner in the third floor pantry (cafeteria), we had a briefing session, a commemorative photo, and completed the first major event of the first day with Dr. Fukui.

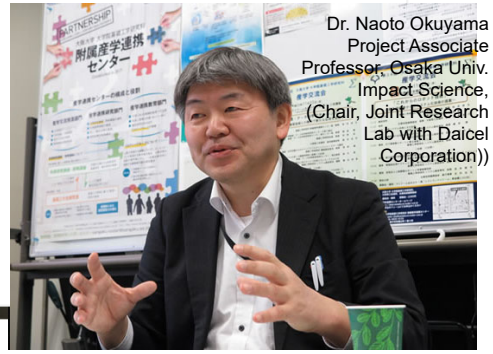
The Institute is...　At the Institute, ...

From "Green and Cultural Kyoto" (KBS)

Interview with Professor Kenichi Fukui

*For copyright reasons, the images are not displayed.

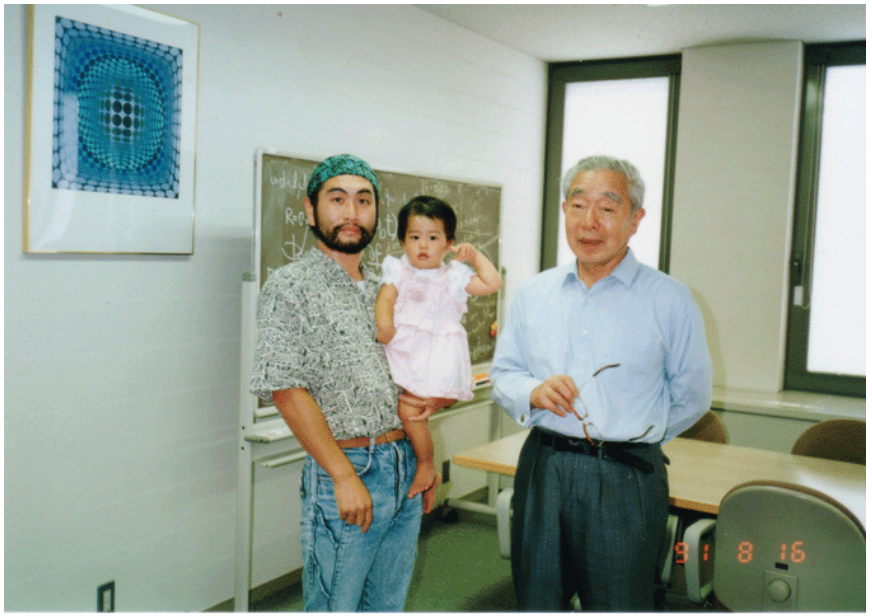
In Laboratory 102 (1991).



Dr. Naoto Okuyama
Project Associate Professor, Osaka Univ.
Impact Science,
(Chair, Joint Research Lab with Daicel Corporation))

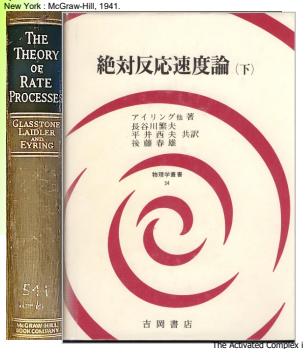
*For copyright reasons, the images are not displayed.

In the director's office (1991)



Research Motivation #1: "The Theory of Rate Processes"

(A standard theory)



The theory of rate process (International chemical series)
by Samuel Glasstone and others.
New York : McGraw-Hill, 1941.

The Activated Complex in Chemical Reactions
by Rudolf A. A. Eyring
Translated by Shigeo Hasegawa, Nishio Hirai, and Haruo Goto
Yoshioka Shoten, 1964

Words in "§8 Reactions in the liquid phase"

"・The treatment of absolute reaction rate theory in solution is, in principle, the same as that in the gas phase. ・・・・ There is some uncertainty, however, concerning partition functions of molecules in the liquid phase, and so it has been found more convenient to treat reactions in solution from a less fundamental point of view". (H. Eyring et al., 1935)

Gas reaction:

$$k = \frac{k_B T}{h} \cdot K^{\neq} = \frac{k_B T}{h} \cdot \frac{F_{\neq}}{F_A F_B \cdots} e^{-E_0/RT}$$

Ratio of partition functions.

Solution reaction (from a less fundamental point of view):

$$k = \frac{k_B T}{h} \cdot K^{\neq} = \frac{k_B T}{h} \cdot \frac{c_M^{\neq}}{c_A c_B \cdots} = \frac{k_B T}{h} \cdot K_0^{\neq} \frac{\alpha_A \alpha_B \cdots}{\alpha_M^{\neq}}$$

Ratio of activity coefficients

True equilibrium constant

<Awareness of the issues>

Solution reactions should also be treated **from a fundamental viewpoint** !!

➔ The Theory of Absolute Reaction Rate using Partition Functions in the Liquid Phase !!

Includes surface reactions and enzymatic reactions!

Research Motivation #2: "Two *T*s: Temperature and Time"

Introduction to Frontier Orbital Theory
by I. Fleming
Supervised by Kenichi Fukui
Translated by Taketo Takeuchi and Shuji Tomoda
Kōdansha, 1978

Chemical Reactions and Electron Orbitals
Kenichi Fukui
Maruzen Co., Ltd., 1976

Fukui Theories { 1. Frontier orbital theory
2. IRC theory

"・In many cases, frontier orbital theory is effective also in solution reactions, but it must sometimes be corrected due to dynamic motion of reactant and solvent molecules. In frontier orbital theory, it is because an orbital is defined by electronic state theory at a static nuclear rearrangement. Moreover, the intrinsic reaction coordinate (IRC) theory is also a theory of the reaction pathway on which a reactant system changes at an infinitely slow speed ("one center of a reaction" (words of Fukui))."
(Monthly Journal "Chemistry" Prof. Fukui's mourning number)

"・Likewise, *solvent effects* (which is usually make themselves felt in the entropy of activation term) are also well known to be part of the explanation of the principal of hard(硬) and soft(軟) acids and bases. ・Arguments based on the interaction of frontier orbitals are powerful, as we shall see, but they must not be taken so far that we forget these very important limitations."

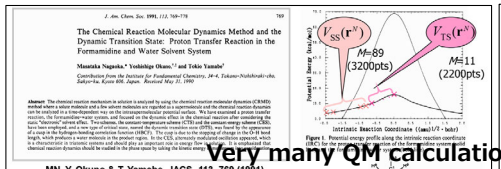
(I. Fleming, "Frontier Orbitals and Organic Chemical Reactions", (1976))

< My Awareness of the Issues >

In both Fukui theories, there is **no explicit dependence** on the concepts of **two "T"s** (*T* and *t*)!!

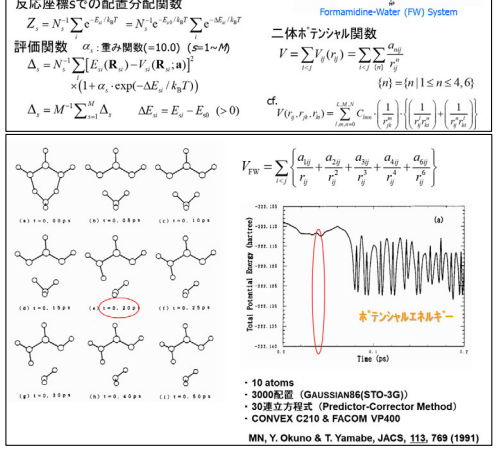
➔ I want to create a theory directly depending on the **two "T"s**!!

Reaction Energy Transfer Mechanisms in Solution Reactions: Heuristic Potential Functions for Chemical Reactions



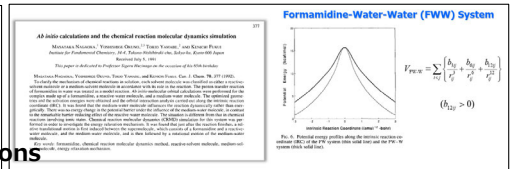
MN, Y. Okuno & T. Yamabe, JACS, 113, 769 (1991)

Very many QM calculations along the reaction coordinate



・10 atoms
・3000配置（GAUSSIAN86(STO-3G)）
・30連立方程式（Predictor-Corrector Method）
・CONVEX C210 & FACOM VP400

MN, Y. Okuno & T. Yamabe, JACS, 113, 769 (1991)



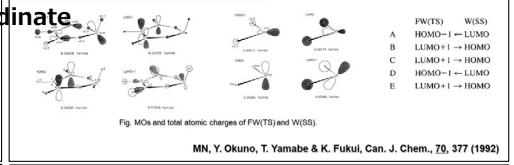
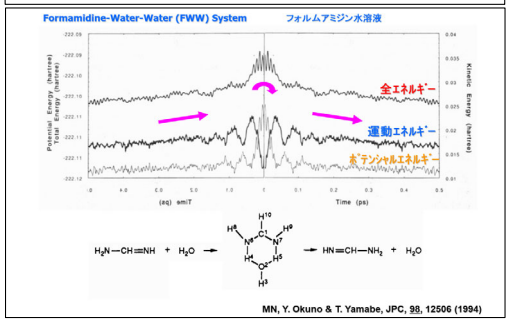


Fig. MOs and total atomic charges of FW(TS) and W(SS).

MN, Y. Okuno, T. Yamabe & K. Fukui, Can. J. Chem., 70, 377 (1992)



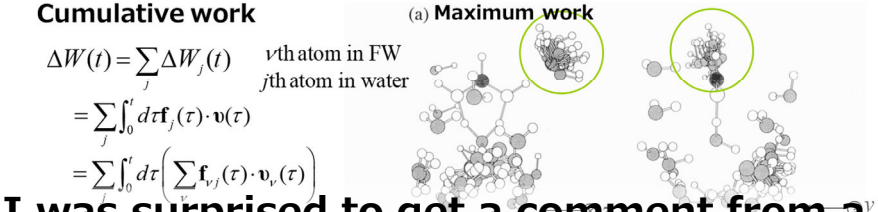
MN, Y. Okuno & T. Yamabe, JPC, 98, 12506 (1994)

Reaction Energy Transfer Mechanisms in Solution Reactions: Heuristic Potential Functions for Chemical Reactions

Reaction energy transfer mechanism in solution reaction (component work analysis)

Cumulative work

$$\Delta W(t) = \sum_j \Delta W_j(t) \qquad \nu\text{th atom in FW},\ j\text{th atom in water}$$
$$= \sum_j \int_0^t d\tau \mathbf{f}_j(\tau)\cdot\mathbf{v}(\tau)$$
$$= \sum_j \int_0^t d\tau \left(\sum_\nu \mathbf{f}_{\nu j}(\tau)\cdot\mathbf{v}_\nu(\tau)\right)$$



I was surprised to get a comment from a reviewer:

"After five papers using one calculation data, that's enough, isn't it?"

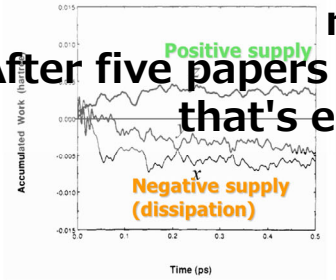
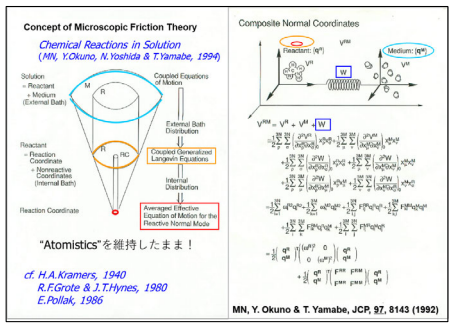


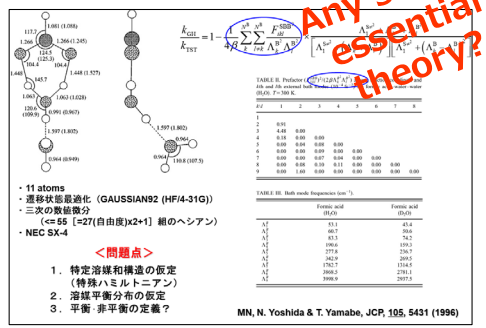
Figure 9. (a) Superimposed pictures of 50 trajectories for the position of the medium water molecule that did the least work on the FW supermolecule in each trajectory. The left and right pictures were drawn with the viewing direction along the z and y axes, respectively. (b) Similar pictures for the medium water molecule that did the most work on the FW supermolecule.

MN, Y. Okuno & T. Yamabe, JPC, 98, 12506 (1994)

Molecular Friction Theory: Chemical Reactions and Brownian Motion

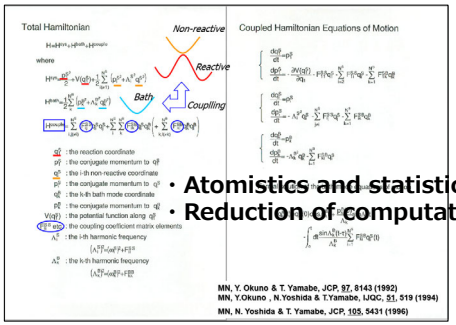


MN, Y. Okuno & T. Yamabe, JCP, 97, 8143 (1992)

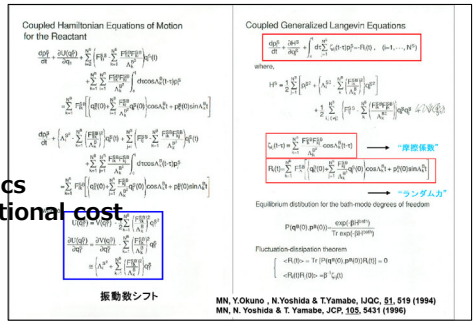


MN, N. Yoshida & T. Yamabe, JCP, 105, 5431 (1996)

Any simple essential theory?



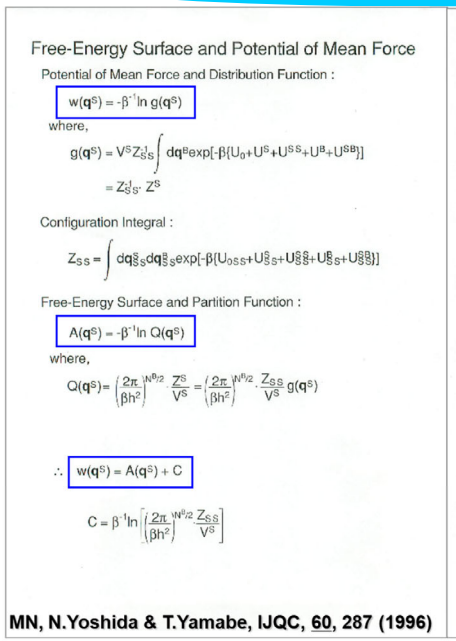
MN, Y. Okuno & T. Yamabe, JCP, 97, 8143 (1992)
MN, Y.Okuno , N.Yoshida & T.Yamabe, IJQC, 51, 519 (1994)
MN, N. Yoshida & T. Yamabe, JCP, 105, 5431 (1996)



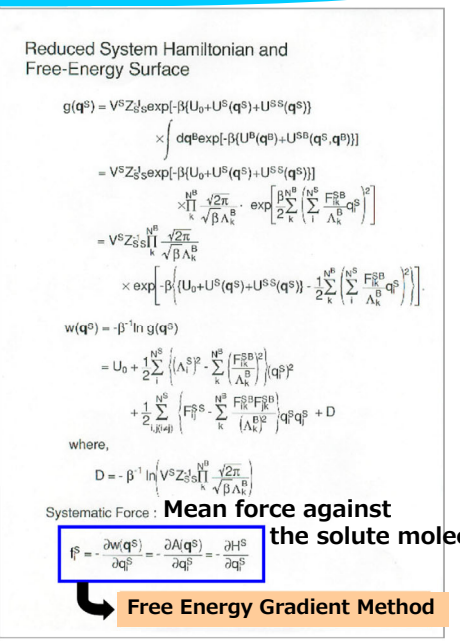
MN, Y.Okuno , N.Yoshida & T.Yamabe, IJQC, 51, 519 (1994)
MN, N. Yoshida & T. Yamabe, JCP, 105, 5431 (1996)

・Atomistics and statistics
・Reduction of computational cost

Molecular Friction Theory and Free Energy Surface



MN, N.Yoshida & T.Yamabe, IJQC, 60, 287 (1996)



Free Energy Gradient Method

Rochester Newhampshire

US-Belgium Summer Tour: ACTC08 & Gordon Conference (Summer'93, BC5)

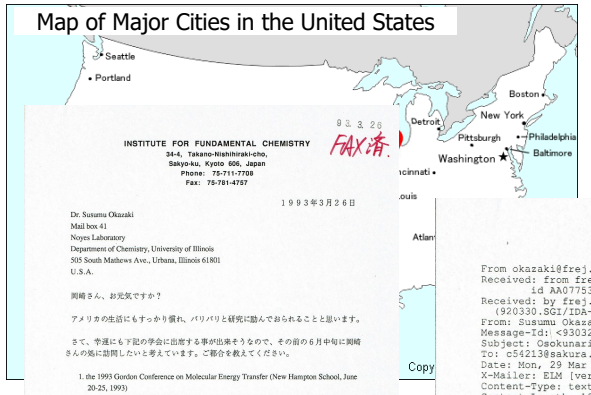
W.A.GoddardIII Lab (CALTECH) Visit (930610-13)

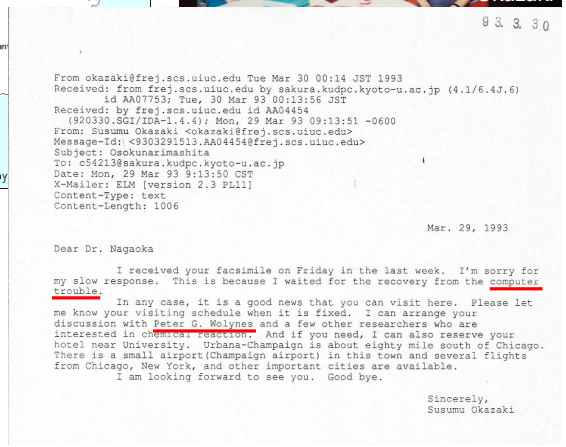
Collapse of the 55-year regime and birth of the Hosokawa administration (general election 930718)

J.T.Hynes Lab (Colorado U@B) Visit (930613-16)

Rochester Newhampshire

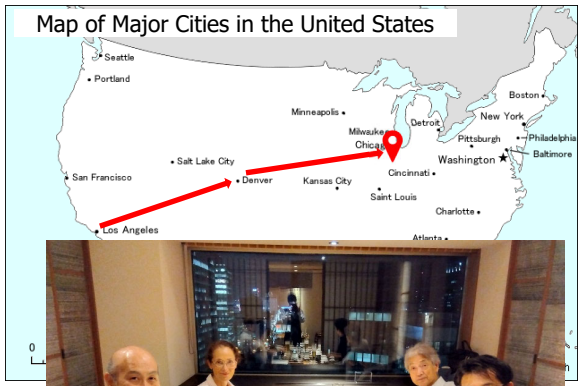
US-Belgium Summer Tour: ACTC08 & Gordon Conference (Summer'93, BC5)





Rochester Newhampshire

US-Belgium Summer Tour: ACTC08 & Gordon Conference (Summer'93, BC5)



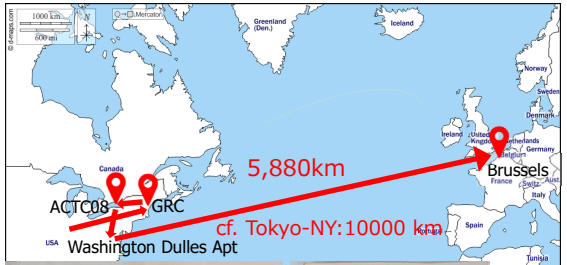
TACC2023(Prof. N.Makri)230905

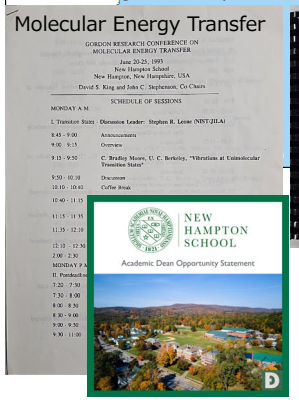
P.Wolynes Lab(Illinois U@UC) Visit 930620 (930616-20)

N.Makri Lab (Illinois U@UC) Visit 930618

Rochester Newhampshire

US-Belgium Summer Tour: ACTC08 & Gordon Conference (Summer'93, BC5)

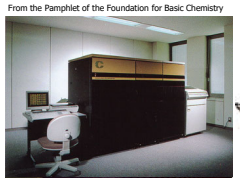




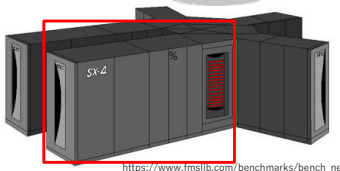
The Arrow of Time Seen from Chaos
Shuichi Tasaki Kōdansha, 2000

I.Pregogine Lab (ULB) Visit (930705-11)

Meeting to NEC Chairman, toward introducing SX-4 System to IFC (950831)



Machine at the time of opening of IFC CONVEX C1-XP



https://www.fmslib.com/benchmarks/bench_nec4.html

T.Sekimoto (関本忠弘)
NEC Chairman(Then)
(IFC trustee)

https://jpn.nec.com/profile/corp/history/pdf/history-120.pdf

https://www.hpcwire.jp/archives/9428

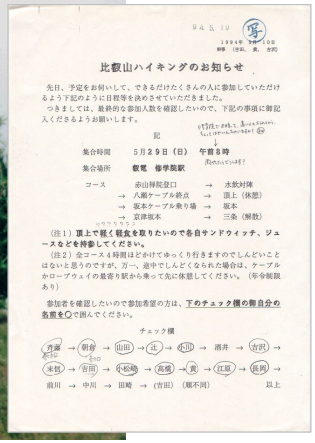
T.Watanabe (渡辺貞)
General manager of HQ of supercomputer sales promotion (Then)
(2009 Japan Academy prize)

Previous Project Leader and Deputy Director, Next Generation Supercomputer Development and Implementation Directorate, RIKEN

"Mt. Hiei Hiking" – At Ropeway Station – (940529, BC4, in 36)

Legendary!

Prof. Fukui always carried a "walking stick" that was given to him by an acharya on Mount Hiei.



比叡山ハイキングのお知らせ

先日、予定をお伺いして、できるだけたくさんの人に参加していただけるよう下記のように日程等を決めさせていただきました。
つきましては、最終的な参加人数を確認したいので、下記の事項に御記入くださるようお願いします。

記

集合時間　5月29日（日）　午前8時
集合場所　叡電　修学院駅
コース　赤山禅院登口 → 水飲対陣 → 八瀬ケーブル終点 → 頂上（休憩） → 坂本ケーブル乗り場 → 坂本 → 京津国本 → 三条（解散）

（注1）頂上で寒く軽食を取りたいので各自サンドウィッチ、ジュースなどを持参してください。
（注2）全コース4時間はどかけてゆっくり行きますのでしんどいことはないと思うのですが、万一、途中でしんどくなられた場合は、ケーブルかロープウェイの最寄り駅から乗って先に休憩してください。（年令制限あり）

参加者を確認したいので参加希望の方は、下のチェック欄の該当分の名前をOで囲んでください。

チェック欄

斉藤 → 朝倉 → 山田 → 庄 → 松川 → 酒井 → 吉沢 → 末松 → 寺田 → 小松崎 → 高橋 → 黄 → 江原 → 長岡 → 前川 → 中川 → 田崎 → （吉田）（順不同）　以上

略歴, Brief History

紀元前BC

77(S52)0322 須坂高等学校卒業
82(S57)0316 京大工石化卒業
84(S59)0314 同院修士 修了
87(S62)0311 同院博士 修了
88(S63)0410 JSPS*研究員(基礎化研)
91(H03)0407 基礎化研 副主任研究員
97(H09)0901 同上 主任研究員
98(H10)0600 同上 退所 (福井先生 他界)

福井先生M2時

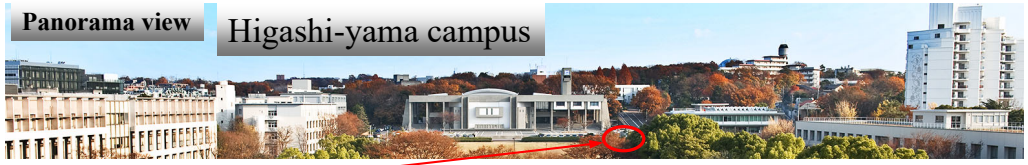
IFC

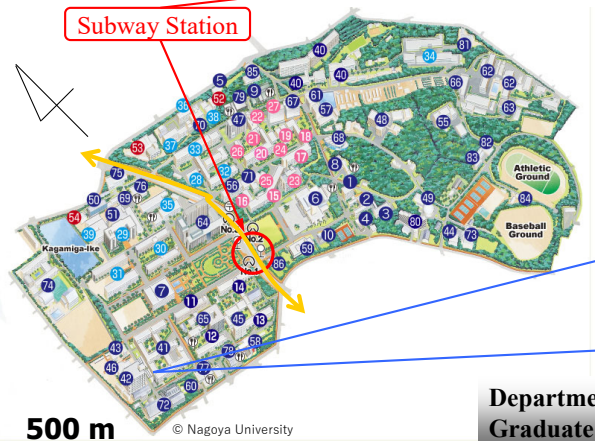
To Nagoya University after ~10 years in IFC.

Autumn

Panorama view

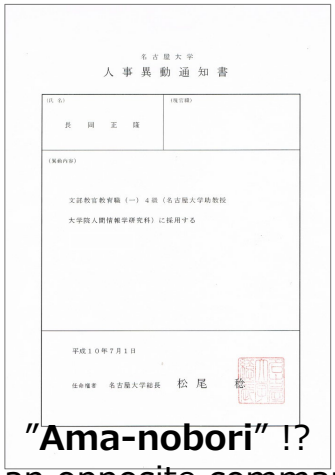
Higashi-yama campus





Department of "Natural Informatics"
Graduate School of "human Informatics"
at that time!

Graduate School of Human Informatics, Nagoya University. Appointed! (‘980701, AD0)


名古屋大学
人事異動通知書

長岡正隆

文部教官教育職（一）４級（名古屋大学助教授
大学院人間情報学研究科）に採用する

平成１０年７月１日

名古屋大学総長　松尾　稔

”Ama-nobori” !?
-- an opposite command from private sector to governmental.

https://www.sun-hp-ibm-sgi-unix-workstations-for-sale.com/wp-content/uploads/1227512570_ban_octane.jpg
https://unixhq.com/systems/sgi-octane/

Ncube Nagaoka Laboratory

Outline

JOURNEY “DEPARTURE”

For copyright reasons, the images are not displayed.

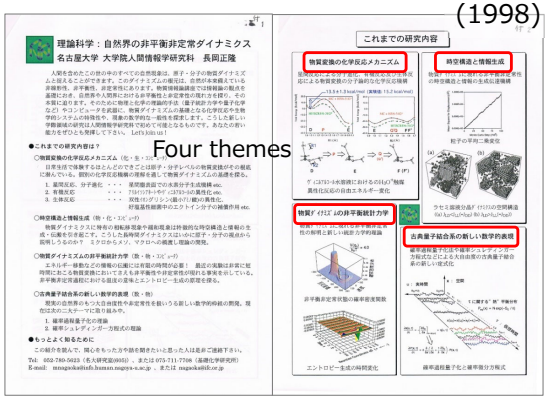
Ncube Nagaoka Laboratory

:01

§4 Nagaoka Lab Starts ! A Departure !?

Graduate School of Human Informatics, Nagoya University. Employed! (‘980701, AD0)

(1998)



Four themes

(1998)
- Chemical reaction mechanism of materials transformation
- Space-time structure and information generation
- Non-equilibrium statistical mechanics of matter dynamics
- New mathematical expressions for classical quantum-coupled systems

(2024)
- From kinetic to nonequilibrium systems
- From isolated reactions to solution chemical reactions
- From elementary reactions to complex chemical reactions
- From molecules to life phenomena
- From parallel computing to multiscale information processing
- Industrial application by interplay between experiments and theoretical calculations

Free energy gradient method (1998)

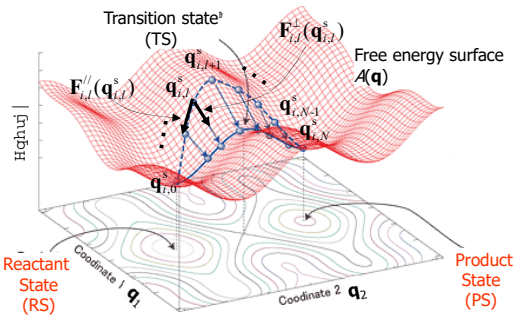
A method to study the shape of molecules and their reactions in solution

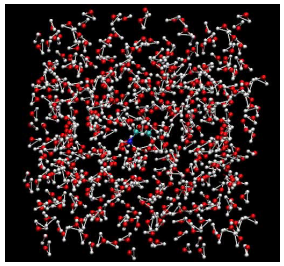
■**A method to find out what shape the molecules in solution**

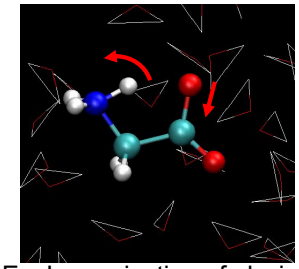
Dyhudjh# irufh# lq#vroxwrq

$$\mathbf{F}^{\mathrm{FE}}_{i,l}(\mathbf{q}^{\mathrm{s}}_{i,l}) = -\frac{\partial A(\mathbf{q}^{\mathrm{s}}_{i,l})}{\partial(\mathbf{q}^{\mathrm{s}}_{i,l})} = -\left\langle \frac{\partial V_{\mathrm{SB}}(\mathbf{q}^{\mathrm{s}}_{i,l})}{\partial(\mathbf{q}^{\mathrm{s}}_{i,l})} \right\rangle_i \approx 0,$$

■**Free energy** $A(\mathbf{q}^{\mathrm{s}}_{i,l}) = -k_{\mathrm{B}}T \ln Z(\mathbf{q}^{\mathrm{s}}_{i,l}) \qquad l = 0, \cdots, N$







Ex. Isomerization of glycine in aqueous solution

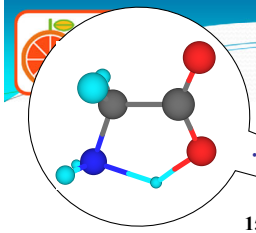
- Q1R10\rvklgd/PQ) #W1\/*Iqwd#M1#F'xdqwxp #F'khp 1/* **435**/#535#4<<;,1#
- Q1Wdnhqdnd/#\1N1wdp xud/#\1Nr|dqr/#W1Dvdgd# #PQ/# *Wkhru1#F'khp 1#Dfwd*/#163/#548 +5344,#

Reaction free energy and activation free energy

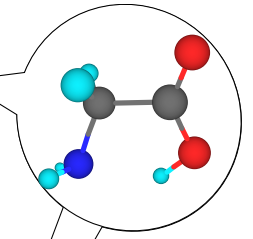
that the free energy gradient method enables to obtain for the first time

Dr. N.Okuyama

- N.O. Yoshida, MN & TY, *J. Chem. Phys.*, **113**, 3519 (2000)
- N.Takenaka, Y.Kitamura, Y.Koyano, T.Asada & MN, *Theor. Chem. Acc.*, **130**, 215 (2011)



Neutral form (NF)



"**Activated state** on the free energy surface"

Activation free energy ΔG_a

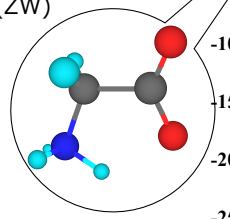
12.3 kcal/mol

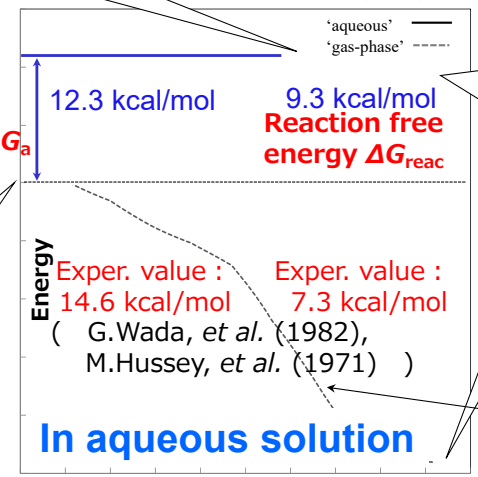
9.3 kcal/mol

Reaction free energy ΔG_{reac}

Strong Stabilization

Zwitterionic form (ZW)





Exper. value : 14.6 kcal/mol (G.Wada, *et al.* (1982), M.Hussey, *et al.* (1971))

Exper. value : 7.3 kcal/mol

In aqueous solution

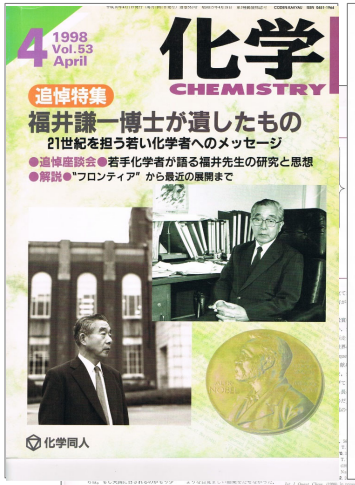
Reaction coordinate (molecular deformation)

Energy curve obtained from previous calculations (Contradictory to experiment!)

Journal『Chemistry(化学)』Memorial Special Issue

– The Legacy of Prof. Fukui –

('98, BC0, in 39)

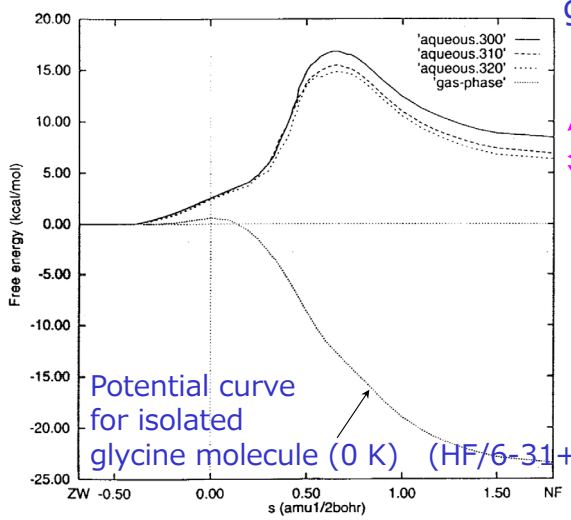


Shogoin Goten-So (Kyoto): The round table meeting was held on Jan. 30, '98.

Young chemists talking about the mentor!

Temperature Dependence of Activation Energy

Temperature dependence can also be obtained from free energy calculations!
(Information that cannot be obtained from QM calculations!)



glycine aqueous solution

300K

310K

320K

Potential curve for isolated glycine molecule (0 K) (HF/6-31+G*)

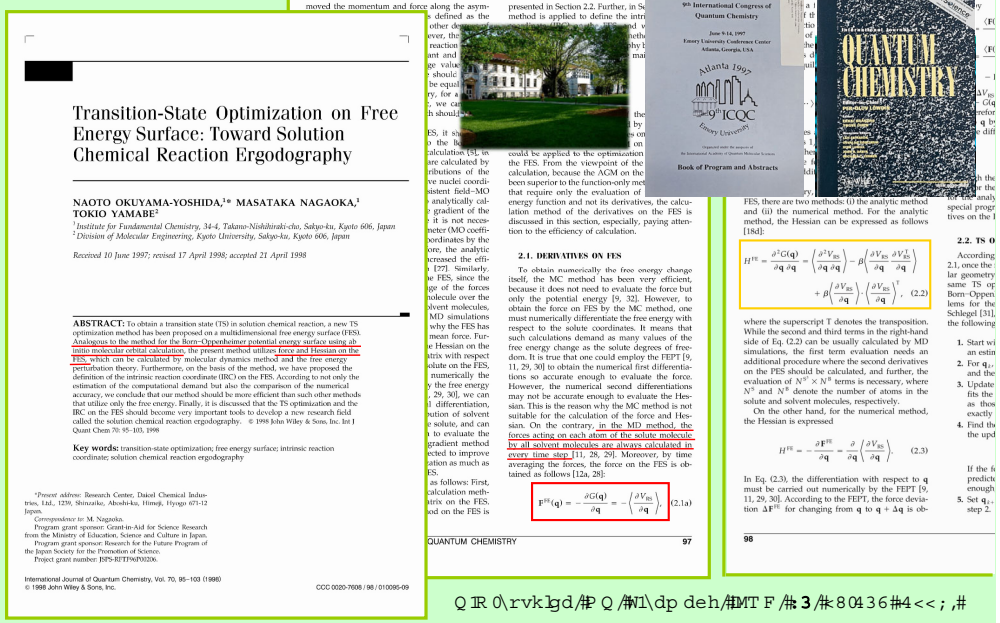
MN, N.Yoshida, T.Yamabe, *JPC* ***A***, **102,** 8202 (1998).

We proposed

Iuhh#Hqhuj|#Judglhqw#Phkrg#4<<;,

FEG Method

Wkh#Rujlgd#Sdshu#Ivvhqwldd#ghdv# #Wkhruhwlfdd#dvvlv#



Transition-State Optimization on Free Energy Surface: Toward Solution Chemical Reaction Ergodography

NAOTO OKUYAMA-YOSHIDA,[1]* MASATAKA NAGAOKA,[1] TOKIO YAMABE[2]

[1] *Institute for Fundamental Chemistry, 34-4, Takano-Nishihiraki-cho, Sakyo-ku, Kyoto 606, Japan*
[2] *Division of Molecular Engineering, Kyoto University, Sakyo-ku, Kyoto 606, Japan*

Received 10 June 1997; revised 17 April 1998; accepted 21 April 1998

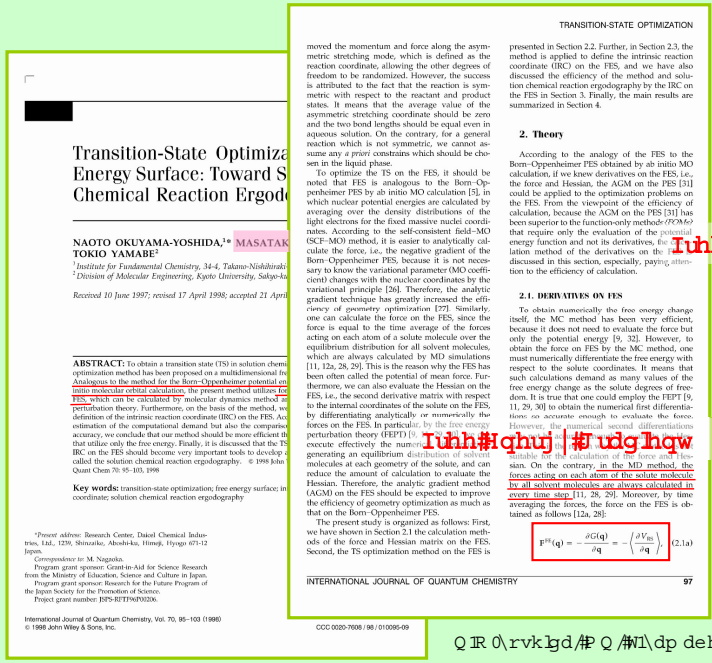
ABSTRACT: To obtain a transition state (TS) in solution chemical reaction, a new TS optimization method has been proposed on a multidimensional free energy surface (FES). Analogous to the method for the Born–Oppenheimer potential energy surface using ab initio molecular orbital calculation, the present method utilizes force and Hessian on the FES, which can be calculated by molecular dynamics method and the free energy perturbation theory. Furthermore, on the basis of the method, we have proposed the definition of the intrinsic reaction coordinate (IRC) on the FES. According to not only the estimation of the computational demand but also the comparison of the numerical accuracy, we conclude that our method should be more efficient than such other methods that utilize only the free energy. Finally, it is discussed that the TS optimization and the IRC on the FES should become very important tools to develop a new research field called the solution chemical reaction ergodography. © 1998 John Wiley & Sons, Inc. Int J Quant Chem 70: 95–103, 1998

Key words: transition-state optimization; free energy surface; intrinsic reaction coordinate; solution chemical reaction ergodography

QIR0\rvkldg#PQ/#W1\dp deh/#DMTF/#k3/#k80436#4<<;,#

Iuhh#Hqhuj|#Judglhqw#Phkrg#4<<;,

FEG Method



Transition-State Optimiza
Energy Surface: Toward S
Chemical Reaction Ergod

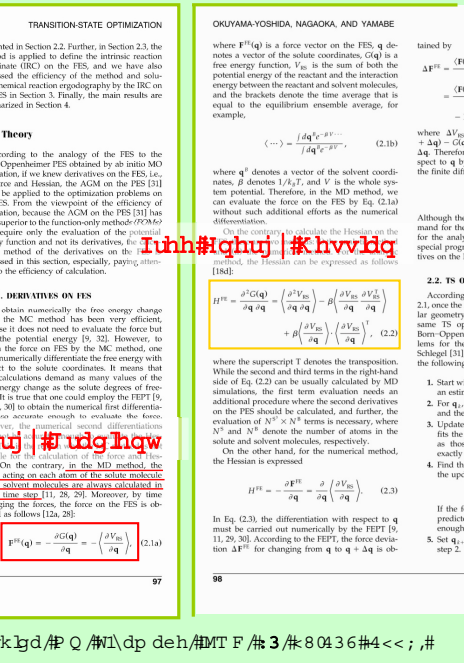
NAOTO OKUYAMA-YOSHIDA,[1]* MASATAK
TOKIO YAMABE[2]

[1] *Institute for Fundamental Chemistry, 34-4, Takano-Nishihiraki*
[2] *Division of Molecular Engineering, Kyoto University, Sakyo-ku*

Received 10 June 1997; revised 17 April 1998; accepted 21 April

Iuhh#Hqhuj|#Khvvldg

Iuhh#Hqhuj|#Judglhqw

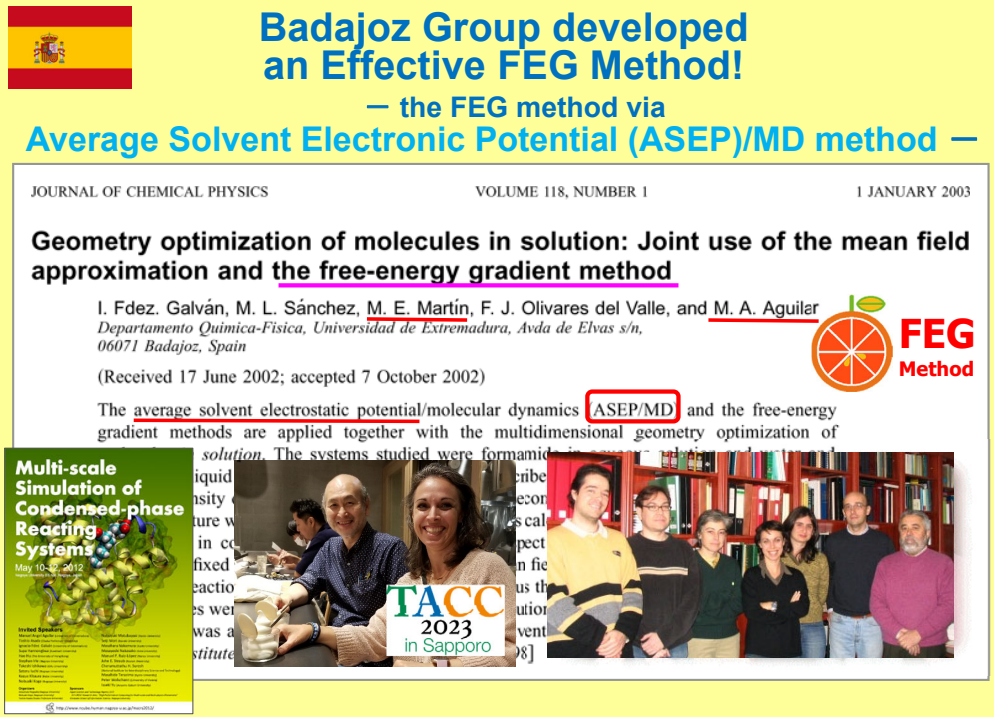


OKUYAMA-YOSHIDA, NAGAOKA, AND YAMABE

QIR0\rvkldg#PQ/#W1\dp deh/#DMTF/#k3/#k80436#4<<;,#

Badajoz Group developed an Effective FEG Method!

— the FEG method via Average Solvent Electronic Potential (ASEP)/MD method —



JOURNAL OF CHEMICAL PHYSICS VOLUME 118, NUMBER 1 1 JANUARY 2003

Geometry optimization of molecules in solution: Joint use of the mean field approximation and the free-energy gradient method

I. Fdez. Galván, M. L. Sánchez, M. E. Martín, F. J. Olivares del Valle, and M. A. Aguilar
Departamento Quimica-Fisica, Universidad de Extremadura, Avda de Elvas s/n, 06071 Badajoz, Spain

(Received 17 June 2002; accepted 7 October 2002)

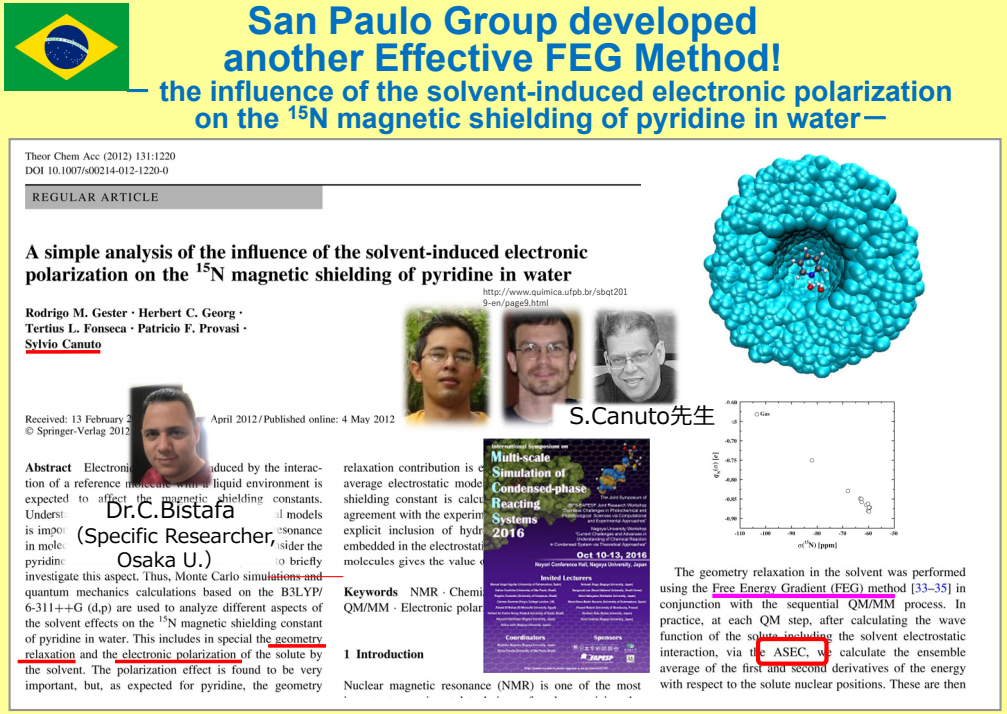
The average solvent electrostatic potential/molecular dynamics (ASEP/MD) and the free-energy gradient methods are applied together with the multidimensional geometry optimization of

FEG Method

F.J. Olivares del Valle and M.A. Aguilar, et al., *J. Chem. Phys.* **118**, 255 (2003)

San Paulo Group developed another Effective FEG Method!

— the influence of the solvent-induced electronic polarization on the ^{15}N magnetic shielding of pyridine in water —



Theor Chem Acc (2012) 131:1220
DOI 10.1007/s00214-012-1220-0

REGULAR ARTICLE

A simple analysis of the influence of the solvent-induced electronic polarization on the ^{15}N magnetic shielding of pyridine in water

Rodrigo M. Gester · Herbert C. Georg · Tertius L. Fonseca · Patricio F. Provasi · Sylvio Canuto

http://www.quimica.ufpb.br/sbqt2019-eng/page9.html

S.Canuto先生

Dr.C.Bistafa
(Specific Researcher, Osaka U.)

Received: 13 February 2012 / April 2012 / Published online: 4 May 2012
© Springer-Verlag 2012

Abstract Electroni… induced by the interac-tion of a reference molecule with a liquid environment is expected to affect the magnetic shielding constants. Understand… models is impor… esonance in mole… sider the pyridine… briefly investigate this aspect. Thus, Monte Carlo simulations and quantum mechanics calculations based on the B3LYP/6-311++G (d,p) are used to analyze different aspects of the solvent effects on the ^{15}N magnetic shielding constant of pyridine in water. This includes in special the geometry relaxation and the electronic polarization of the solute by the solvent. The polarization effect is found to be very important, but, as expected for pyridine, the geometry relaxation contribution is e… average electrostatic mode… shielding constant is calcu… agreement with the experim… explicit inclusion of hydr… embedded in the electrostati… molecules gives the value …

Keywords NMR · Chemi… QM/MM · Electronic polar…

1 Introduction

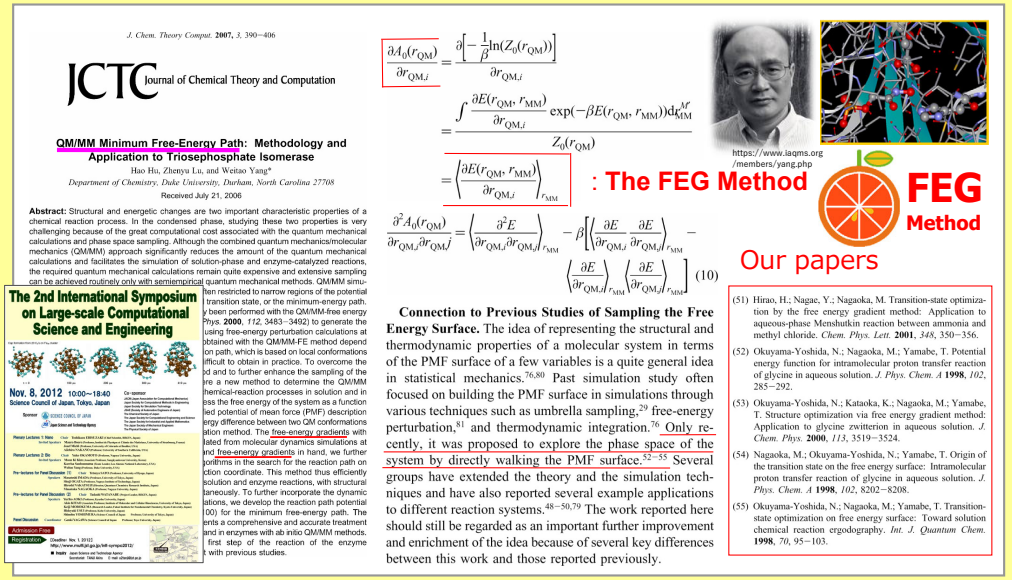
Nuclear magnetic resonance (NMR) is one of the most

The geometry relaxation in the solvent was performed using the Free Energy Gradient (FEG) method [33–35] in conjunction with the sequential QM/MM process. In practice, at each QM step, after calculating the wave function of the solute including the solvent electrostatic interaction, via the ASEC, we calculate the ensemble average of the first and second derivatives of the energy with respect to the solute nuclear positions. These are then

R.M.Gester, H.C.Georg, T.L.Fonseca, P.F.Provasi, S.Canuto, *TCA*, **131**, 1220 (2012)

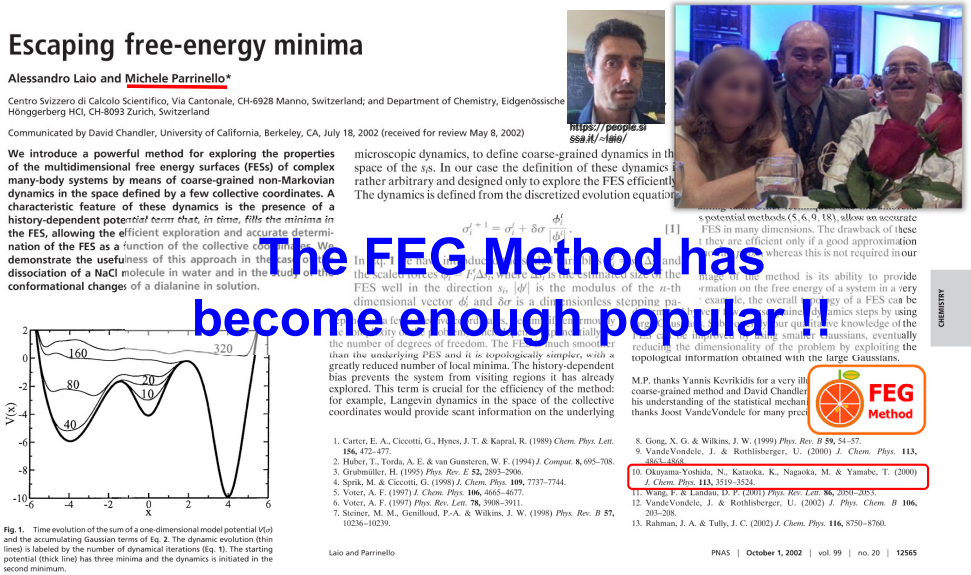
Yang's Group developed also a FEG Method !

— the FEG method via QM/MM Minimum Free-Energy Path (QM/MM-MFEP) Method



H. Hu, Z. Lu and W. Yang, *J. Chem. Theory and Comput.* **3**, 390 (2007)

FEG Method must have influenced the of "Meta-dynamics method" !?



A. Laio and M. Parrinello, *PNAS*, **99**, 12562 (2002)

Brief Personal History

AD

98(H10)07 00 Assoc. Prof. of GS. of Human Informatics, NU — Change to NU

10 JST*Computational Science and Technology Specific Research and Development Promotion Project: **ACT-JST** "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems"

*JST: Japan Science and Tech Corporation

Birth of Lab Ncube !

Birth of "Three "Non"s" !!

02(H14)03 04 Int. Conf. CRN³ (Clarifying Non-equilibrium non-stationarity characteristic of chemical reaction phenomena) (Grant-in-aid: C)

02(H14)09 Prof. (Human Info)

03(H15)04 05 Prof. (Info. Sci.)

04(H16)04 06 21st Century COE "Computational Science Frontiers"

06(H18)10 08 JST*Core Research for Evolutionary Science and Technology: **CREST** "Research Development of Multiscale Simulation of Aggregation Reaction Systems"

07(H19)04 09 Minor ailment

08(H20)12 10 **"Ready-to-Use Manual for Molecular Simulation Beginners"** Published !

12(H24)05 14 MSCRS2012 (JST International)

13(H25)10 15 JST*Core Research for Evolutionary Science and Technology: **CREST** "Establishment of Computational Molecular Tech-nology towards Macro-scopic Chemical Phenomena"

14(H26)04 16 StudyCamp2014

15(H27)12 17 PACIFICHEM2015

16(H28)04 18 MSCRS2016 (JSPS Japan-Brazil+NU)

17(H29)04 19 Prof. (Fac. and GS. of Informatics)

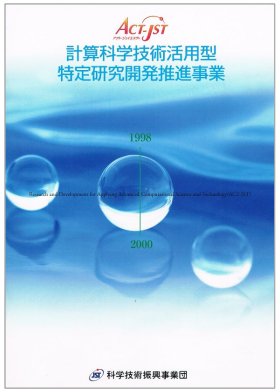
18(H30)09 20 Kanreki (60th BD)

20(R02)12 22 PACIFICHEM2020

23(R05)03 25 StudyCamp2022

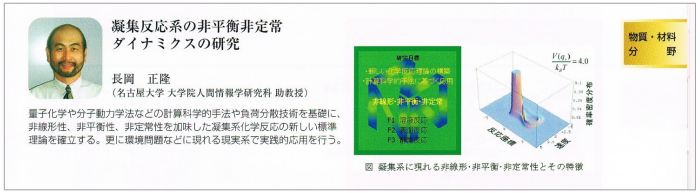
ACT-JST "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems" **Accepted!!**

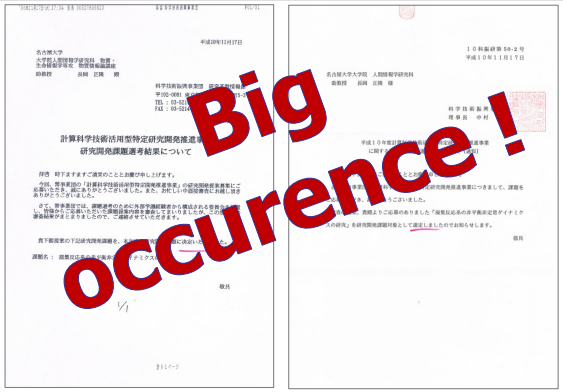
('981117, AD0)



Dr. Masaki Sasai, who encouraged me to apply (Professor at the Graduate School of Human Informatics at Nagoya University at the time)

http://www.iar.nagoya-u.ac.jp/~oldsite/2003PBF/Sasai.html

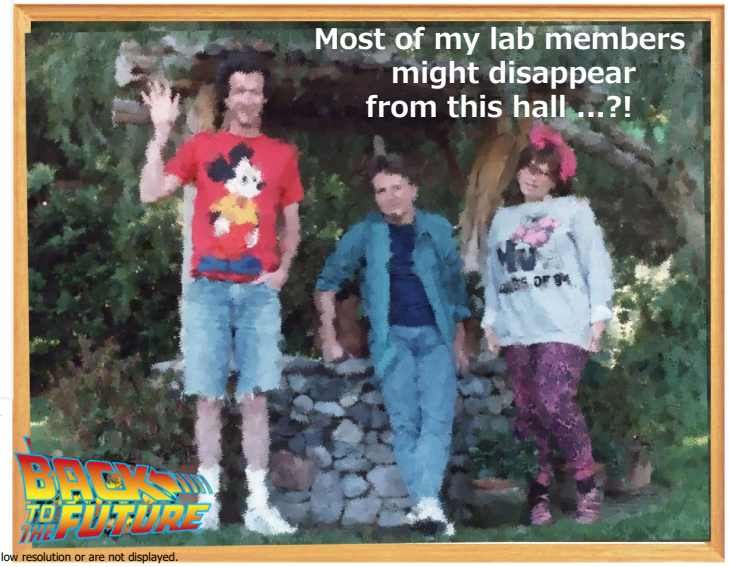




Big occurence !

ACT-JST "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems" **Accepted!!** ('981117, AD0)

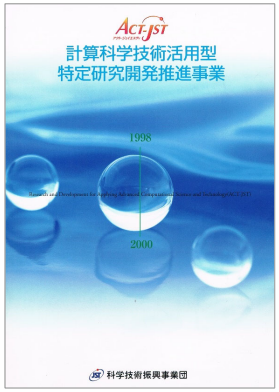
If this project had not been adopted, history would have changed...



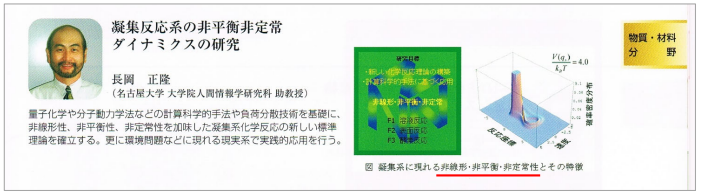
"Back to the Future"
(R. Zemeckis, 1985)

For copyright reasons, some images are shown in low resolution or are not displayed.

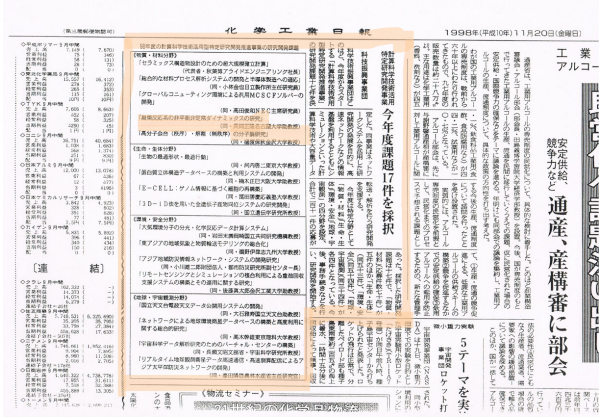
ACT-JST "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems" **Accepted!!** ('981117, AD0)



Japan Science and
Technology "Corporation"



Research Period : 3 years
Research Fee : ~150,000 kYen



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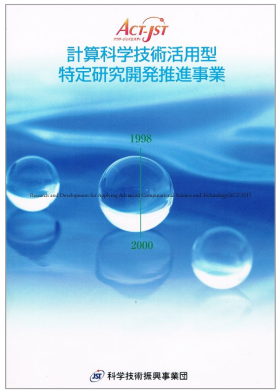

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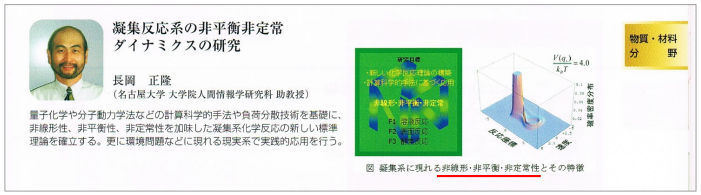
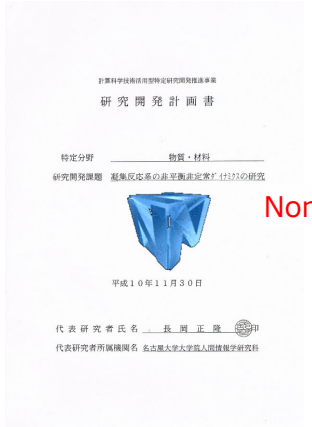
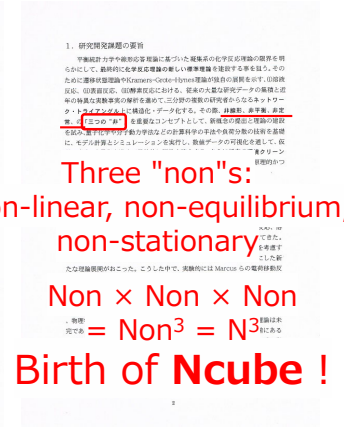
Technology "Corporation"







Three "non"s:
Non-linear, non-equilibrium,
non-stationary

Non × Non × Non
= Non^3 = N^3

Birth of **Ncube** !

ACT-JST "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems" **Accepted!!** ('981117, AD0)

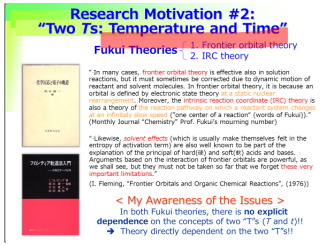
PC Cluster (DEC (COMPAQ))

SiliconGraphics
Computer Systems

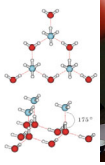
Origin200 (SiliconGraphics)

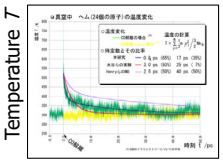
"A Year-End Party 1999" in Sakae ('99, AD1)

ACT-JST "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems" **Accepted!!** ('981117, AD0)

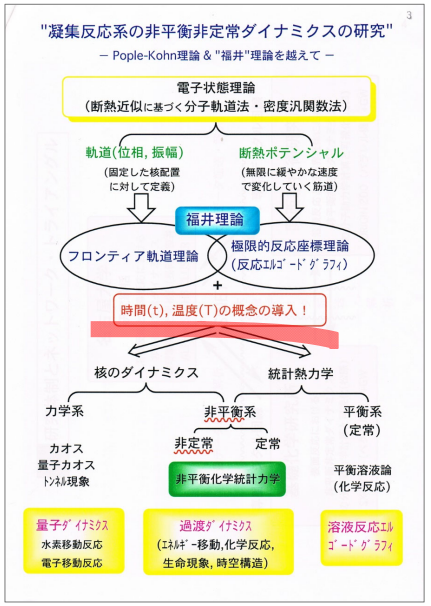


Dr. T.Okamoto (then M2, now at HPC Systems) worked on ***T*** and ***t*** research from a theoretical and informatics point of view.



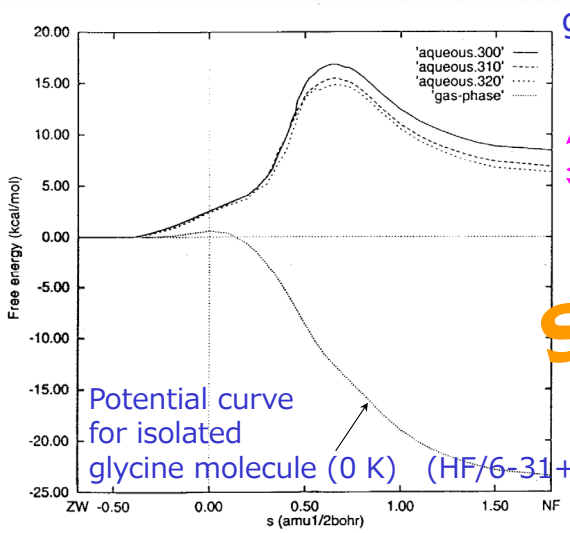


Dr. I.Okazaki (then PD, now a lecturer at Hirosaki University) and Dr. Y.Hara (then M2, now a senior researcher at AIST) who practiced ***T*** and ***t*** research.



Temperature Dependence of Activation Energy

Temperature dependence can also be obtained from free energy calculations!
(Information that cannot be obtained from QM calculations!)



glycine aqueous solution
300K
310K
320K

Potential curve for isolated glycine molecule (0 K) (HF/6-31+G*)

Shown again!

MN, N.Yoshida, T.Yamabe, *JPC* ***A***, **102,** 8202 (1998).

Brief Personal History

AD	
77(S52)03	Grad. Suzaka High Schl
82(S57)03	Grad. Fac. Eng. KU.
84(S59)03	Completed MC, KU.
87(S62)03	Completed DC, KU.
88(S63)04	JSPS*Fellow (IFC)
91(H03)04	Deputy Chief RO (IFC)
93(H05)06	**US-Belgium Summer Tour**
97(H09)09	Chief RO (IFC)
98(H10)01	Leaving (Prof. Fukui Passed away)
98(H10)0700	Assoc. Prof. of GS. of Human Informatics, NU (Change to NU)
10	JST*Computational Science and Technology Specific Research and Development Promotion Project: **ACT-JST** "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems"
02(H14)0304	Birth of "Three "Non"s" !! **Int. Conf.** CRN³ (Clarifying Non-equilibrium non-stationarity characteristic of chemical reaction phenomena) (Grant-in-aid: C)
02(H14)09	Prof. (Human Info)
03(H15)0405	Prof. (Info. Sci.)
04(H16)0406	21st Century COE "Computational Science Frontiers"

*JST: Japan Science and Tech Corporation

Birth of Lab Ncube !

Prof. Fukui awarded N!

*JSPS: Japan Society for the Promotion of Science

AD	
06(H18)1008	JST*Core Research for Evolutionary Science and Technology: **CREST** "Research Development of Multiscale Simulation of Aggregation Reaction Systems"
07(H19)0409	Minor ailment
08(H20)1210	**"Ready-to-Use Manual for Molecular Simulation Beginners"** Published !
12(H24)0515	MSCRS2012 (JST International)
13(H25)1016	JST*Core Research for Evolutionary Science and Technology: **CREST** "Establishment of Computational Molecular Tech-nology towards Macroscopic Chemical Phenomena"
14(H26)0417	StudyCamp2014
15(H27)1218	PACIFICHEM2015
16(H28)0419	MSCRS2016 (JSPS Japan-Brazil+NU)
17(H29)0420	Prof. (Fac. and GS. of Informatics)
18(H30)0921	Kanreki (60th BD)
20(R02)1223	PACIFICHEM2020
23(R05)0325	StudyCamp2022

Brief Personal History

AD		
77(S52)03	Grad. Suzaka High Schl	
82(S57)03	Grad. Fac. Eng. KU.	
84(S59)03	Completed MC, KU.	Prof. Fukui awarded Nobel
87(S62)03	Completed DC, KU.	*JSPS: Japan Society for the Promotion of Science
88(S63)04	JSPS*Fellow (IFC)	
91(H03)04	Deputy Chief RO (IFC)	
93(H05)06	**US-Belgium Summer Tour**	
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98(H10)01	Leaving (Prof. Fukui Passed away)	
98(H10)07	Assoc. Prof. of GS. of Human Informatics, NU	Change to NU
00 10	JST*Computational Science and Technology Specific Research and Development Promotion Project: **ACT-JST** "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems"	*JST: Japan Science and Tech Corporation
Birth of Lab Ncube !	Birth of "Three "Non"s" !!	
02(H14)03	**Int. Conf.** CRN³ (Clarifying Non-equilibrium non-stationarity characteristic of chemical reaction phenomena) (Grant-in-aid: C)	04
02(H14)09	Prof. (Human Info)	
03(H15)04	Prof. (Info. Sci.)	05
04(H16)04	21st Century COE "Computational Science Frontiers"	06
06(H18)10	JST*Core Research for Evolutionary Science and Technology: **CREST** "Research Development of Multiscale Simulation of Aggregation Reaction Systems"	08
07(H19)04	Minor ailment	09
08(H20)12	**"Ready-to-Use Manual for Molecular Simulation Beginners"** Published !	10
12(H24)05	MSCRS2012 (JST International)	15
13(H25)10	JST*Core Research for Evolutionary Science and Technology: **CREST** "Establishment of Computational Molecular Tech-nology towards Macro-scopic Chemical Phenomena"	16
14(H26)04	StudyCamp2014	17
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17(H29)04	Prof. (Fac. and GS. of Informatics)	20
18(H30)09	Kanreki (60th BD)	21
20(R02)12	PACIFICHEM2020	23
23(R05)03	StudyCamp2022	25

Brief Personal History

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97(H09)09	Chief RO (IFC)	
98(H10)01	Leaving (Prof. Fukui Passed away)	
98(H10)07	Assoc. Prof. of GS. of Human Informatics, NU	Change to NU
00 10	JST*Computational Science and Technology Specific Research and Development Promotion Project: **ACT-JST** "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems"	*JST: Japan Science and Tech Corporation
Birth of Lab Ncube !	Birth of "Three "Non"s" !!	
02(H14)03	**Int. Conf.** CRN³ (Clarifying Non-equilibrium non-stationarity characteristic of chemical reaction phenomena) (Grant-in-aid: C)	04
02(H14)09	Prof. (Human Info)	
03(H15)04	Prof. (Info. Sci.)	05
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CREST "Research Development of Multiscale Simulation of Aggregation Reaction Systems

- Coarse-graining of large-scale atomic information, development of reconstruction techniques and coarse-graining theory " ('06, AD08)

Core **R**esearch for **E**volutional **S**cience and **T**echnology
(Japan Science and Technology Agency)

Research Director

Prof. G.Yagawa
(Professor Emeritus, The University of Tokyo)
(Former Professor, Toyo University)

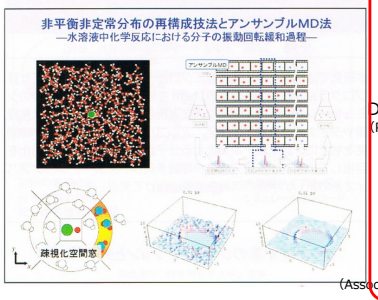
Area Advisor

Dr. T. Watanabe
(Project Leader, RIKEN Next Generation Supercomputer Development and Implementation Directorate at the time) and 9 others

Research Period : 5.5 years
Research Fee : ~300,000 kYen

凝集反応系マルチスケールシミュレーションの研究開発
—大規模原子情報の疎視化・再構成技法・疎視的理論の開発—
長岡 正隆（名古屋大学大学院情報科学研究科 教授）

溶液、表面、生体高分子の非経験的分子動力学（MD）シミュレーションで得た原子情報を疎視化・再構成する凝集反応系マルチスケールシミュレーションを実現します。具体的には、1）疎視化技法と疎視化発展方程式、2）最大エントロピー原理による非定常状態の再構成技法、3）分子軌道法とMD法とを繋ぐQM／MMインターフェースを研究開発し、最終的には個別事例に適用して、凝集反応系マルチスケールシミュレーション実用化基盤を確立します。




Dr. T.Okamoto
(HPC systems)


Dr. M.Takayanagi
(Assoc. prof., Shiga U.

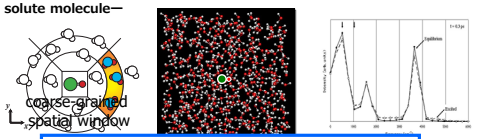

Dr. N.Yamamoto
(Prof., Chiba I.Tech.)


Dr. I. Yu
(Assoc. prof. Maebashi IT)

"Study on Multiscale Simulation of Aggregation Reaction Systems
- Coarse-graining of large-scale atomic information, development of reconstruction techniques and coarse-graining theory –"

Ncube Nagaoka Laboratory

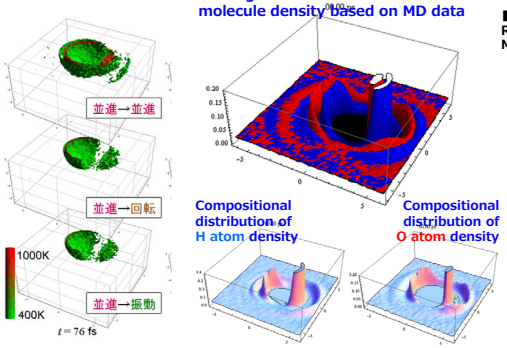
■ **Observation of Vibrational Relaxation Process of HF Molecules in Aqueous Solution** —Real space non-equilibrium non-stationary distribution appearing in a group of water molecules around a solute molecule—



From individual molecular vibrational energy to spatiotemporal distribution of solvent temperature

2011 "Hatsumode" Atami Jingu（110114）

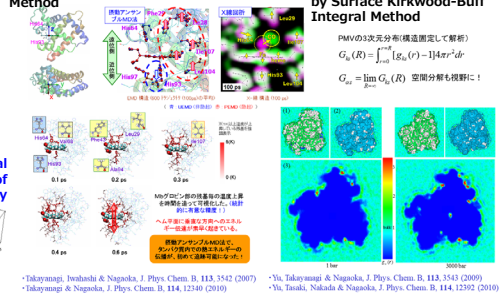
Original distribution of water molecule density based on MD data



Compositional distribution of H atom density

Compositional distribution of O atom density

■ **Prediction of the initial Process of Relaxation by the Perturbed Ensemble MD Method**



■ **Microscopic Elucidation of Protein Volume Para-doxes by Surface Kirkwood-Buff Integral Method**

・Takayanagi, Iwahashi & Nagaoka, J. Phys. Chem. B, **113**, 3542 (2007)
・Takayanagi & Nagaoka, J. Phys. Chem. B, **114**, 12340 (2010)
・Yu, Takayanagi & Nagaoka, J. Phys. Chem. B, **113**, 3543 (2009)
・Yu, Tasaki, Nakada & Nagaoka, J. Phys. Chem. B, **114**, 12392 (2010)

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03(H15)0405	Prof. (Info. Sci.)
04(H16)0406	21st Century COE "Computational Science Frontiers"
06(H18)1008	JST*Core Research for Evolutionary Science and Technology: **CREST** "Research Development of Multiscale Simulation of Aggregation Reaction Systems"
07(H19)0409	Minor ailment
08(H20)1210	**"Ready-to-Use Manual for Molecular Simulation Beginners" Published !**
12(H24)0514	MSCRS2012 (JST International)
13(H25)1015	JST*Core Research for Evolutionary Science and Technology: **CREST** "Establishment of Computational Molecular Tech-nology towards Macroscopic Chemical Phenomena"
14(H26)0416	StudyCamp2014
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*JST: Japan Science and Tech Corporation

Prof. Fukui awarded NU

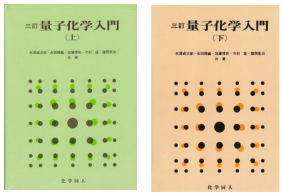
*JSPS: Japan Society for the Promotion of Science

Change to NU

Birth of Lab Ncube !

"Ready-to-Use Manual for Molecular Simulation Beginners" Published !（'081210, AD10）

Kōdansha Scientific, 2008



"*Introduction to Quantum Chemistry*" compiled by Prof. Morokuma and others in Fukui Lab.

Writing Process Chart

Construction of "Dragon" at Suzaka High School, my alma mater (NHK Ningen Documentary: **"Make a dragon that strikes the sky"** (2006.9.8)
https://www.dailymotion.com/video/x26ar32

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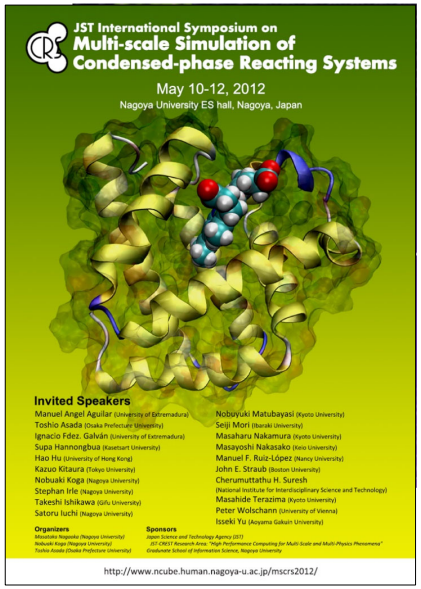
Change to NU

Birth of Lab Ncube !

JST International Symposium MSCRS2012

"Multi-scale Simulation of Condensed-phase Reacting Systems" ('12, AD17)



Ncube Nagaoka Laboratory

Outline

JOURNEY "DEPARTURE"

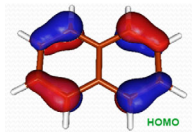
For copyright reasons, the images are not displayed.

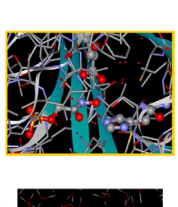
Ncube Nagaoka Laboratory

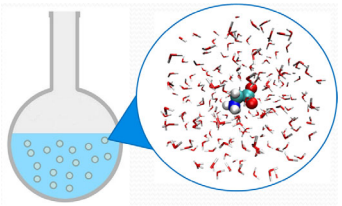
:01

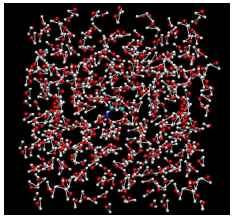
§ 5 Evolving ! Toward the Complexity

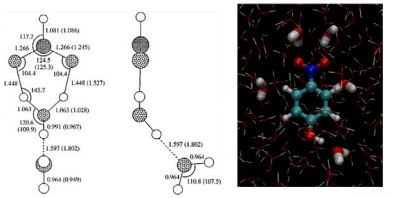
Single molecules, elementary reactions have been primarily studied so far!

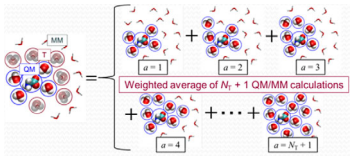


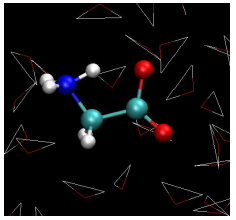


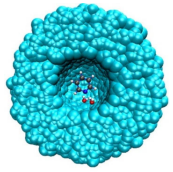


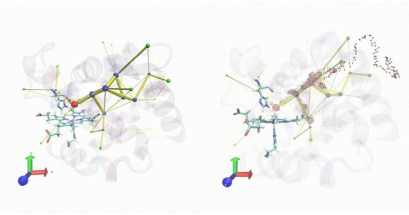








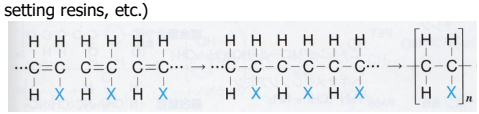




The World is Full of Complex "Materials"!

-Our lives are surrounded by compounds of complex composition-

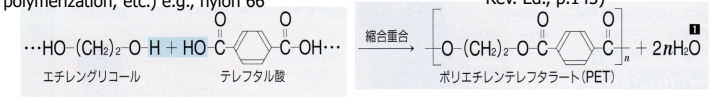
■Synthetic resins (plastics) (thermoplastic resins, thermo-setting resins, etc.)



Polyethylene

©写真AC

■Synthetic fibers (by condensation polymerization, addition polymerization, etc.) e.g., nylon 66



"Basic Chemistry, Newly Rev. Ed." and "Chemistry, Newly Rev. Ed." (Jikkyo Publishing) (2018)

Polyethylene terephthalate (PET) etc.

UNIQLO Heattech Commercial
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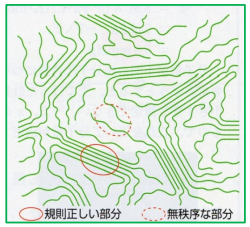
some images are not displayed.

UNIQLO

Although the reaction equation is neat and tidy, in fact, polymer compounds have complex structures!



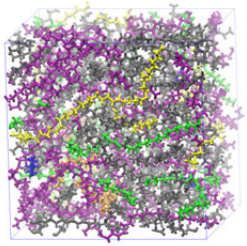
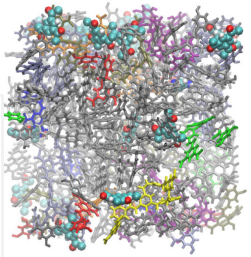


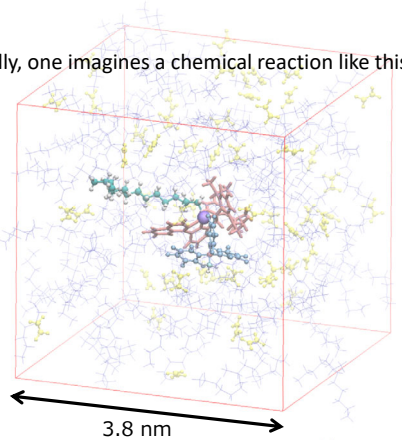
Fig. Structure of polymeric compounds in solids(Chemistry II, Newly Rev. Ed., p.143)



The image of a "chemical reaction"!?

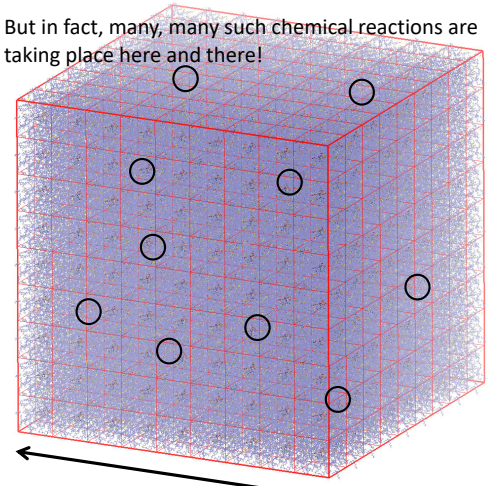
A complex reaction system is a system of random variables!

Usually, one imagines a chemical reaction like this!



3.8 nm
3,706 atomic system
(=126x1+6x60+23x140)
(Hf catalyst 1+ ethene 60 + heptane 140)

But in fact, many, many such chemical reactions are taking place here and there!



34.2 nm
(This system includes **2,701,674** atoms)
(ethene 43,740, heptane 102,060)

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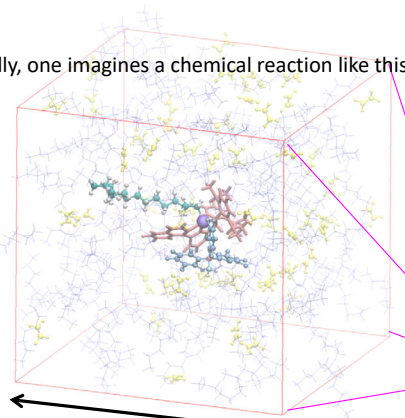

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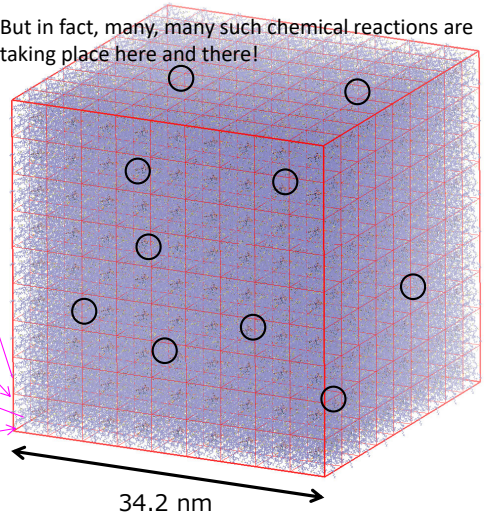

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Red Moon Method -Hybrid MC/MD Reaction Method-

~Molecular simulation to study compounds of complex components~

RM Method

"A hybrid MC/MD reaction method with Rare event-driving Methodology of necessity"
MN, Y.Suzuki, T.Okamoto, N.Takenaka, *Chem. Phys. Lett.*, **583**, 80 (2013)

Red Moon Method

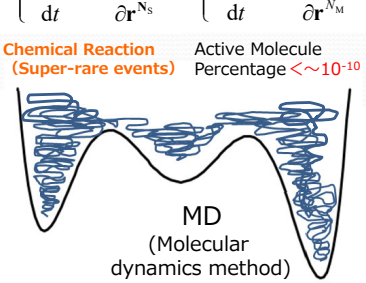
··· A new simulation method

Previous simulation methods

Newton's equations of motion:

$$\begin{cases} \dfrac{d\mathbf{r}^{N_S}}{dt} = \dfrac{\partial H}{\partial \mathbf{p}^{N_S}} \\ \dfrac{d\mathbf{p}^{N_S}}{dt} = -\dfrac{\partial H}{\partial \mathbf{r}^{N_S}} \end{cases} \quad \begin{cases} \dfrac{d\mathbf{r}^{N_M}}{dt} = \dfrac{\partial H}{\partial \mathbf{p}^{N_M}} \\ \dfrac{d\mathbf{p}^{N_M}}{dt} = -\dfrac{\partial H}{\partial \mathbf{r}^{N_M}} \end{cases}$$

Chemical Reaction (Super-rare events)　Active Molecule Percentage $<\sim 10^{-10}$



It doesn't happen very often!

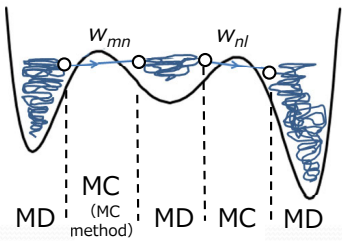
Active molecule 1
vs.
Inert molecules **10 billion**

- A Hybrid MC/MD Reaction Method
- Transition rate (Metropolis method):

$$w_{mn} = \min\left\{1, \exp\left[-\beta \Delta U_{mn}\right]\right\}$$

- Reaction energy difference:

$$\Delta U_{mn} = \Delta U_{mn}^{\mathrm{MM}} + \Delta U_{mn}^{0}$$



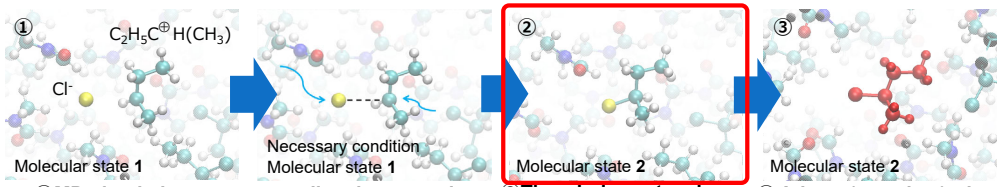
To solve the "master equation,"

"Red Moon Method" uses the MC and MD methods repeatedly!

EXAMPLE

(R)-$C_2H_5CH(CH_3)Cl$ ⇌ $C_2H_5C^{\oplus}H(CH_3)$ + Cl^- ⇌ (S)-$C_2H_5CH(CH_3)Cl$

***Intrinsic* MD(iMD) simulation for chemical bond formation from Bu^+ and Cl^- to (R)-2-chlorobutane (2CLRBTN)**

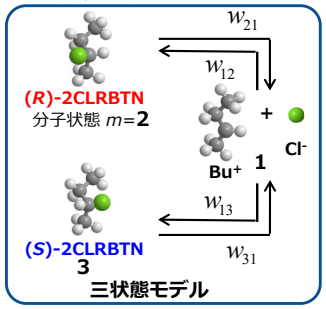


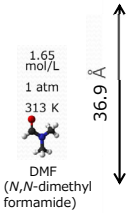
①MD simulations are run until a given atomic pair satisfies the necessary conditions.

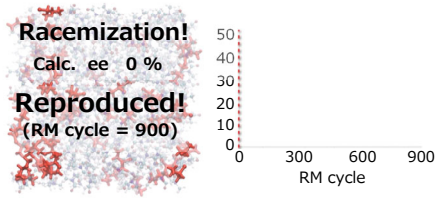
②The whole system is made to react virtually while relaxing.

③Adopt (or reject) that reaction step under the Metropolis scheme.

■反応スキーム







0 RM cycle

Red: (*R*)-2-Chlorobutane (**50** molecules (Initial state))
Blue: (*S*)-2-Chlorobutane (**0** molecules (Initial state))
Black: 2-Butyl cation, Cl^-anion (Each **0** molecule) (Initial state)
Ball&Stick(Skyblue): DMF(**350** molecules) (Initial state)

・MN, Y.Suzuki, T.Okamoto, N.Takenaka, *Chem. Phys. Lett.*, **583**, 80 (2013)

Industry-Academia Collaboration Practicum (A) No. 1

One of the education to acquire the ability to understand and analyze the problems and demands of the real world

('12, AD17)

N.Ohnishi, Previous Dean of Grad, School of Info. Sci (2010-12)

■ **Curriculum of the Graduate School of Information Science**

In addition to a curriculum that enables students to acquire a common foundation and academic foundations of information science, the curriculum incorporates industry-academia collaboration, including research internships, off-campus training, and **industry-academia collaboration training**, in order to acquire the ability to understand and analyze real world problems and demands.

Dr. Y.Suzuki

(1)産学連携実習科目A, B(博士前期課程)

共同研究などを主体として、実習担当教員、企業担当者、学生が一体となって、研究開発を実施する科目。

履修希望者は、指導教員の承諾のもと、履修申請を行い、教務入試委員会で承諾する。

要件:① 企業担当者をプロジェクトリーダとする組織とする。

② 実習時間数の要件を満足する(最低30hx単位数、Aは通年4単位、Bは半年2単位。)

③ 定期的に(1カ月に1度程度)実習状況報告、方向性の検討のための3者によるミーティングを行う。

④ 終了時に発表会を行い、教務入試委員会に実績報告を提出する。通年の場合は中間発表も行う。発表会の開催は研究科内に周知する。

⑤ 単位認定は実習担当教員が行う。

平成23年12月8日

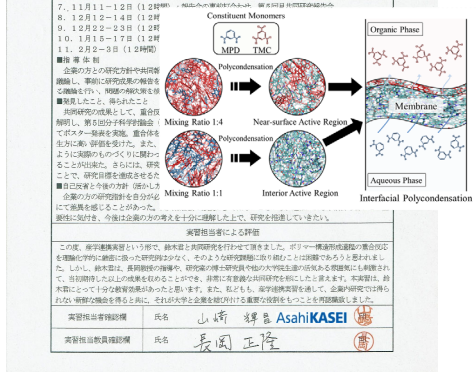
情報科学研究科

産学連携実習科目 中間発表会について

専攻	発表者	テーマ	日 時	場 所	指導教員
複雑系科学専攻 M2	鈴木 雄一	膜ポリマーの構造と機能に関する分子科学的手法の研究	12月22日(木) 13:30~14:30	情報科学研究科棟 第2講義室	長岡 正隆

実習担当者評認欄 氏名 山崎 輝昌 AsahiKASEI

実習担当教員確認欄 氏名 長岡 正隆



Ncube Nagaoka Laboratory

"Red Moon" in Manchester !

RM Method

Brief Personal History

AD		
77(S52)03		Grad. Suzaka High Schl
82(S57)03		Grad. Fac. Eng. KU.
84(S59)03		Completed MC, KU.
87(S62)03		Completed DC, KU.
88(S63)04		JSPS*Fellow (IFC)
91(H03)04		Deputy Chief RO (IFC)
93(H05)06		**US-Belgium Summer Tour**
97(H09)09		Chief RO (IFC)
98(H10)01		Leaving (Prof. Fukui Passed away)
98(H10)07	00	Assoc. Prof. of GS. of Human Informatics, NU
	10	JST*Computational Science and Technology Specific Research and Development Promotion Project: **ACT-JST** "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems"
02(H14)03	04	Birth of "Three "Non"s" !! **Int. Conf.** CRN³ (Clarifying Non-equilibrium non-stationarity characteristic of chemical reaction phenomena) (Grant-in-aid: C)
02(H14)09		Prof. (Human Info)
03(H15)04	05	Prof. (Info. Sci.)
04(H16)04	06	21st Century COE "Computational Science Frontiers"
06(H18)10	08	JST*Core Research for Evolutionary Science and Technology: **CREST** "Research Development of Multiscale Simulation of Aggregation Reaction Systems"
07(H19)04	09	Minor ailment
08(H20)12	10	**"Ready-to-Use Manual for Molecular Simulation Beginners"** Published !
12(H24)05	15	MSCRS2012 (JST International)
13(H25)10	16	JST*Core Research for Evolutionary Science and Technology: **CREST** "Establishment of Computational Molecular Tech-nology towards Macroscopic Chemical Phenomena"
14(H26)04	17	StudyCamp2014
15(H27)12		PACIFICHEM2015
16(H28)04	19	MSCRS2016 (JSPS Japan-Brazil+NU)
17(H29)04	20	Prof. (Fac. and GS. of Informatics)
18(H30)09	21	Kanreki (60th BD)
20(R02)12	22	PACIFICHEM2020
23(R05)03	25	StudyCamp2022

Prof. Fukui awarded N!

*JST: Japan Science and Tech Corporation

*JSPS: Japan Society for the Promotion of Science

Change to NU

Birth of Lab Ncube !

CREST "Establishment of Computational Molecular Technology towards Macroscopic Chemical Phenomena" adopted! ('13, AD16)

Core **R**esearch for **E**volutional **S**cience and **T**echnology
Japan Science and Technology Agency

Research Director

新機能創出を目指した分子技術の構築
Establishment of Molecular Technology towards the Creation of New Functions

Prof. Hisashi Yamamoto
(Emeritus Prof. at Nagoya U., Chubu U.)
https://www.jst.go.jp/crest/mt/supervisor/

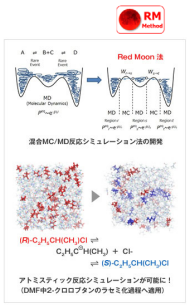
Dr. M.Takayanagi
(Assoc. prof., Shiga U.)

Dr. S.Xing

Research Period : 5.5 years
Research Fee : ~300,000 kYen

概要 Outline

本研究では、多数の分子が集まった"分子凝集状態"で起こる複合化学反応の制御を目指します。そのために、ミクロに見ると非常に稀にしか起こらない化学反応（超希少現象）を、原子・分子情報を保持したまま扱う、新しい計算分子技術を創り上げ、科学技術イノベーションを図ります。具体的には、凝集系化学反応の立体化学制御と超ナノ階層集合体の構造制御を実現して、新機能材料を設計・創成します。最終的に、マクロ化学現象をシミュレーションの計算分子技術の汎用環境を実験家と協働して提供したいと夢見ています。



Research Project Outline
This project aims at control of complex chemical reactions in the "molecular aggregation state" where a large number of molecules literally gather. For the purpose, new "computational molecular technology" will be developed, keeping atomic and molecular information, to treat such chemical reactions that do occur very rarely from the microscopic viewpoint (i.e., super-rare phenomena), then leading to a technology innovation. Realizing the stereochemical control of aggregation-state chemical reactions and the structural control of super-nano scale aggregates, new functional materials will be designed and created. We are dreaming to finally offer the general-purpose environment of the "computational molecular technology" of macroscopic chemical phenomena simulation, through collaboration with experimentalists.

Dr. Y. Suzuki

Dr. S. S.Saha
(Assoc. prof. TDB U.)

Dr. Y. Kitamura
(Assi. Prof. Shizuoka U.)

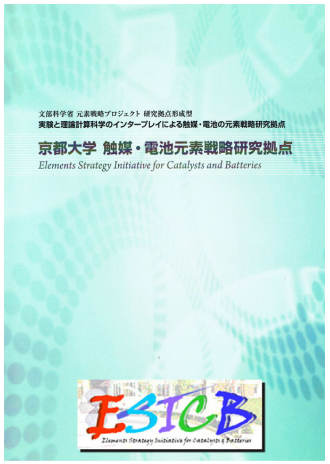
Dr. C.Bistafa
(PD. Osaka U.)

MEXT Participation in "Elements Strategy" & "Post "K"" Projects (Since '12, AD15)

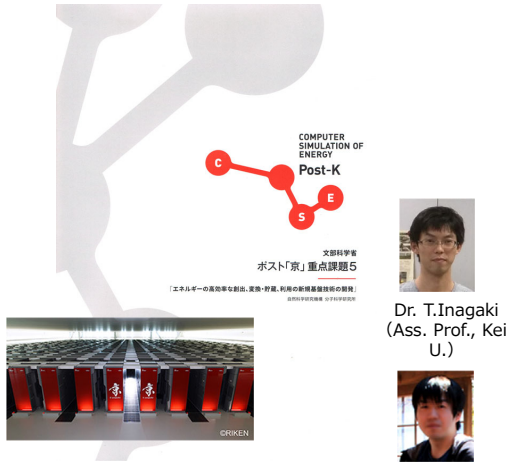
文部科学省（MEXT）
Ministry of **E**ducation, **C**ulture, **S**ports, **S**cience and **T**echnology

Dr. N.Takenaka
(Lecturer, U. Tokyo)

Dr. A.Bouibes
(Assoc. Prof. INSA Toulouse)



Elements Strategy Initiative for Catalysts and Batteries



Post "K" Project

Dr. T.Inagaki
(Ass. Prof., Keio U.)

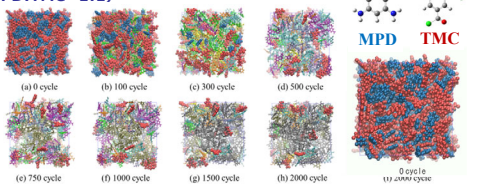
Mr. T.Fujie

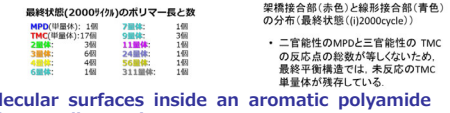
CREST "Molecular Technology" "Establishment of Computational Molecular Technology towards Macroscopic Chemical Phenomena"

Ncube Nagaoka Laboratory

Interfacial Polycondensation Reaction -Aromatic Polyamide Synthetic Fibers-

■Polymerization process and molecular distributions (MPD:TMC=1:1)

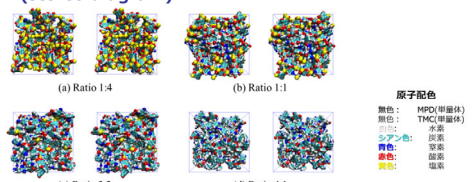




架橋接合部（赤色）と線形接合部（青色）の分布（最終状態((i)2000cycle)）

・二官能性のMPDと三官能性の TMCの反応点の総数が等しくないため，最終平衡構造では，未反応のTMC単量体が残存している．

■Molecular surfaces inside an aromatic polyamide film (stereo diagram)



比率1：1、3：2の膜では、非常に多くの高分子集合体からなる密な部分が形成されている。密な高分子ネットワークが形成。少ない集合体ポア。（実験と一致）

・Y. Suzuki, Y. Koyano, M. Nagaoka, *J. Phys. Chem. B*, **119**, 6776 (2015).

■Degree of polymer cross-linking (DPC) and atomic composition ratio

Early successes

表. 計算値と実験値との比較

	Present[a]				Experiment[b]	
	Ratio 1:4	Ratio 1:1	Ratio 3:2	Ratio 4:1	XPS	RBS
DPC	94.3 ± 0.1	96.9 ± 0.1	99.0 ± 0.0	100.0 ± 0.0	91.7 ± 3.9	96.2 ± 0.2
%C	67.8 ± 0.1	71.6 ± 0.1	73.6 ± 0.1	74.9 ± 0.0	71.0 ± 1.6	71.0 ± 1.2
%O	25.7 ± 0.1	18.6 ± 0.1	14.2 ± 0.1	9.4 ± 0.0	26.2 ± 1.7	17.4 ± 0.4
%N	6.5 ± 0.1	9.9 ± 0.1	12.2 ± 0.0	15.6 ± 0.0	2.8 ± 1.7	11.5 ± 0.6

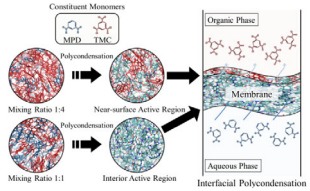
[a]Ratio=*n*(MPD):*n*(TMC)。5個のサンプルの平均値。
[b]それぞれ、X線光電子分光法(XPS)と、ラザフォード後方散乱法(RBS)による結果。

□ 比率１:４の結果はX線光電子分光法（XPS）による実験値に近い傾向を示していることが分かった。

□ 一方、比率１:１の計算結果は、組成比及び高分子架橋度ともに、ラザフォード後方散乱法（RBS）による実験値と良い一致を示した。

（ Red Moon法 のマクロ化学現象シミュレーション手法としての意義と価値）

■Conceptual diagram and interpretation of atomic composition ratios

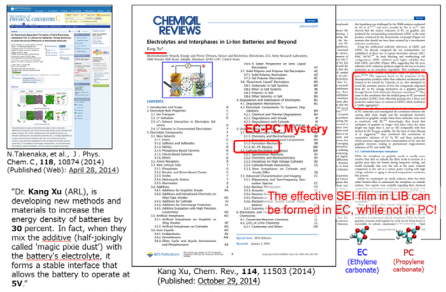


FT-30膜は、コーティング層と一部の活性層とからなる近表面活性領域（表面から~36 nmまで）と膜構造の大半を占める活性層からなる内部活性領域（36nm以上から~92nmまで）とで構成されている。

Toward Structural Elucidation of the Solid-Electrolyte Interphase in Secondary Batteries and its Higher Capacity

RM Method

■Unraveling the EC-PC Mystery



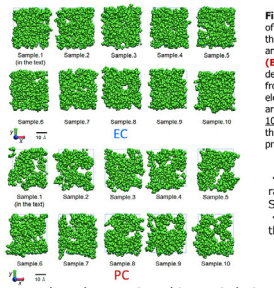


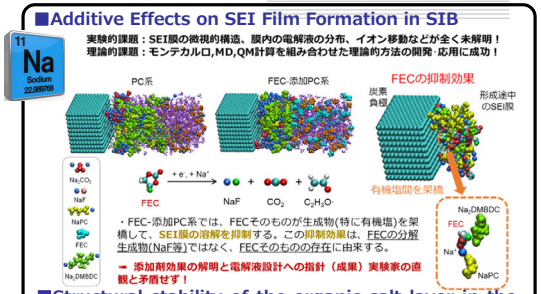
Figure. Front view snapshots of the interface structures of the **EC-based SEI film (Top)** and the **PC-based SEI film (Bottom)** (visualized in the depth 0 < z < 20 Å of the view from the side of bulk electrolyte). These structures are obtained from the different 10 initial configurations, where the sample 1 is shown in the previous panel.

・In PC case, there are rather larger voids in the SEI layer.
・In contrast, in EC case, there is not.

・N. Takenaka, Y. Suzuki, H. Sakai, MN, *J. Phys. Chem. C.*, **118**, 10874 (2014)

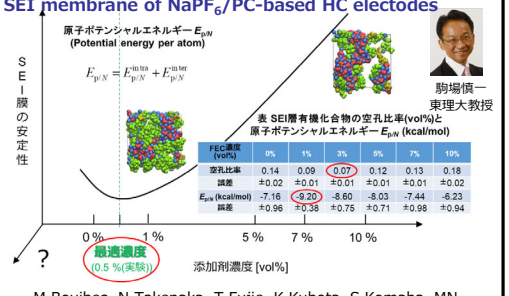
■Additive Effects on SEI Film Formation in SIB

実験的課題：SEI膜の微視的構造、膜内の電解液の分布、イオン移動などが全く未解明！
理論的課題：モンテカルロ,MD,QM計算を組み合わせた理論的方法の開発・応用に成功！



・FEC-添加PC系では、FECそのものが生成物(特に有機塩)を架橋して、SEI膜の溶解を抑制する。この抑制効果は、FECの分解生成物(NaF等)ではなく、FECそのものの存在に由来する。
➡ 添加剤効果の解明と電解液設計への指針（成果）実験家の直観と矛盾せず！

■Structural stability of the organic salt layer in the SEI membrane of $NaPF_6$/PC-based HC electodes



駒場慎一
東理大教授

・M.Bouibes, N.Takenaka, T.Fujie, K.Kubota, S.Komaba, MN, *ACS Appl. Mat. Intrface,* **10**, 28525 (2018)

“The Joys, Angers, Sorrows, and Pleasures of Researchers in Informatics” (Planned) Prof. Arita

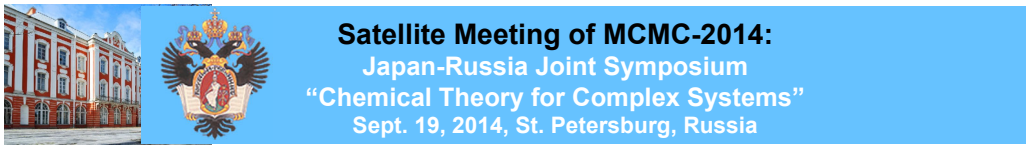
-When is the time you felt "joy" (or was you felt most joy)?

I was given a bold challenge (a **"problem" outside of the problem!?**), "Can't your Red Moon method be used for "Li-ion batteries?" I was given this bold challenge by an outside expert in a different speciality. I felt joy when I realized that, as I worked recklessly on it, I managed to produce results that led to the elucidation of the "EC-PC Mystery"!.

-When is the time you feel "fun" (or was you had the most fun)?

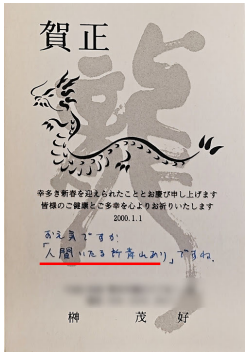
At the Ncube training camp "Study Camp", current students and graduates present their new developments with surprising ingenuity and novel sense. At the compeers, they smile and enthusiastically discuss their hardships! When I am on the sidelines of it all (a regular summer session that is not during the Corona disaster)

Moscow Symposium “Chemical Theory for Complex Systems” (’14, AD17)



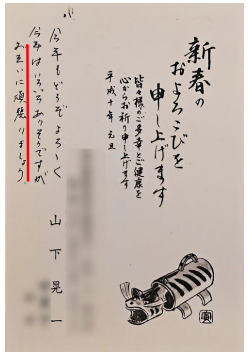
「人間至る所青山あり」(a proverb)
“There's room for us all in the world”

「お互いに頑張りましょう」
“Let's do our best for each other”

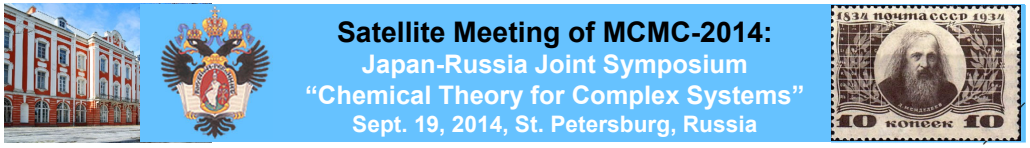


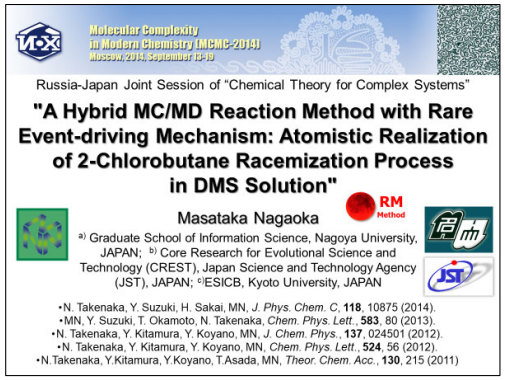
New Year's cards

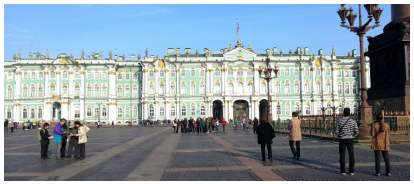
Get-together party at the symposium



Moscow Symposium “Chemical Theory for Complex Systems” (’14, AD17)





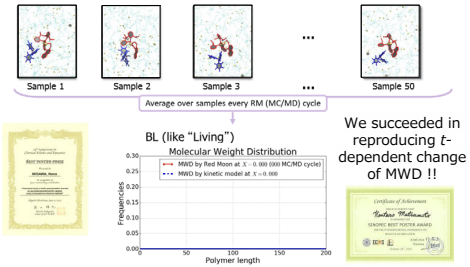


CREST “Molecular Technology” “Establishment of Computational Molecular Technology towards Macroscopic Chemical Phenomena”

Ncube Nagaoka Laboratory

Catalytic Polymerization and Radical Polymerization -Polyolefin Resins-

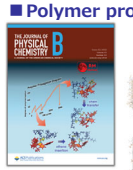
■ **Time-dependent change of molecular weight distribution (mass-average molecular weight)**



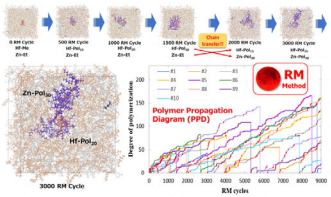
We succeeded in reproducing *t*-dependent change of MWD !!

・M.Matsumoto, M.Takayanagi, Y.Suzuki, N.Koga, MN, *J. Comp. Chem.*, **40**, 421 (2019).

■ **Polymer propagation diagram (PPD)** ⋯ Monomer component ratios can be calculated!

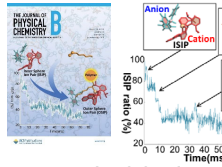


Ethene insertion reduces the steric hindrance to reopen the active site.



・S.Kanesato, K.Yasoshima, N.Misawa, K.Matsumoto, Y.Suzuki, N.Koga, MN, *J. Phys. Chem. B*, **127**, 7735 (2023).

■ **Polymerization reaction mechanism Two different time scales**



A computational chemistry method was established to simulate copolymerization reactions and chain transfer polymerization in the 1-octene/ethene system.

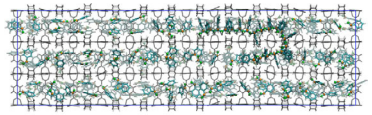
・N.Misawa, K.Matsumoto, Y.Suzuki, S.Saha, N.Koga, MN, *J. Phys. Chem. B*, **127**, 1209 (2023).

■ **Styrene polymerization observed between MOF channels**

Computed St_{20} polymer sequence:
rrrrrrrrmmrmmrmrmmr

At the 1st time of opening the revolving “BDC-doors” (RM cycle 101)
At the 2nd time of opening the revolving “BDC-doors” (RM cycle 170)

tacticity mm : rr : mr (m) = **18** : 41 : 41 (18 (38))
cf. Exp. 16 : 43 : 41 (38)[a] ($P_m = mm + 0.5 \cdot mr$)



・Z.Rao, M.Takayanagi, MN, *J. Phys. Chem. B*, **126**, 5343 (2022)

eHfCat_OCT_ETH_3.mp4
A chain transfer reaction occurs at 1124 RM cycle for #9.

Brief Personal History

AD		
77(S52)03	Grad. Suzaka High Schl	
82(S57)03	Grad. Fac. Eng. KU.	
84(S59)03	Completed MC, KU.	
87(S62)03	Completed DC, KU.	
88(S63)04	JSPS*Fellow (IFC)	
91(H03)04	Deputy Chief RO (IFC)	
93(H05)06	**US-Belgium Summer Tour**	
97(H09)09	Chief RO (IFC)	
98(H10)01	Leaving (Prof. Fukui Passed away)	
98(H10)07	Assoc. Prof. of GS. of Human Informatics, NU	Change to NU
00 10	JST*Computational Science and Technology Specific Research and Development Promotion Project: **ACT-JST** "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems"	
02(H14)03	Birth of "Three "Non"s" !!	Birth of Lab Ncube !
04	**Int. Conf.** CRN³ (Clarifying Non-equilibrium non-stationarity characteristic of chemical reaction phenomena)	
02(H14)09	(Grant-in-aid: C) Prof. (Human Info)	
03(H15)04	Prof. (Info. Sci.)	
05 04(H16)04 06	21st Century COE "Computational Science Frontiers"	

*JST: Japan Science and Tech Corporation

Prof. Fukui awarded Nobel Prize

*JSPS: Japan Society for the Promotion of Science

AD		
06(H18)10	08	JST*Core Research for Evolutionary Science and Technology: **CREST** "Research Development of Multiscale Simulation of Aggregation Reaction Systems"
07(H19)04	09	Minor ailment
08(H20)12	10	**"Ready-to-Use Manual for Molecular Simulation Beginners"** Published !
12(H24)05	15	MSCRS2012 (JST International)
13(H25)10	16	JST*Core Research for Evolutionary Science and Technology: **CREST** "Establishment of Computational Molecular Tech-nology towards Macroscopic Chemical Phenomena"
14(H26)04	17	StudyCamp2014
15(H27)12		PACIFICHEM2015
16(H28)04	19	MSCRS2016 (JSPS Japan-Brazil+NU)
17(H29)04	20	Prof. (Fac. and GS. of Informatics)
18(H30)09	21	Kanreki (60th BD)
20(R02)12	22	PACIFICHEM2020
23(R05)03	25	StudyCamp2022

StudyCamp2014 (Gujo-Kogen Highland) (郡上高原)(Aug.25-27, 2014)

1st StudyCamp was held inspired by "OntakeMeeting2014" (Mar. 31-Apr. 1, 2014)

"StudyCamp" Starts ! ('14, AD17)

Trying on Making Soba Noodle in Gujyo!

Brown udon ?!

Waiting for "soba" boiling!

@StudyCamp Aug.26, 2014

StudyCamps

SC2015 (Gero-Onsen, Gifu)
(下呂温泉)(Aug.24-25)
Profs. Shinoda, Hatanaka


SC2016 (Gujo-Hachiman, Gifu)
(郡上八幡)(Sept.4-5)
Profs. Takahashi, Muraoka


SC2017 (Suwa, Nagano)
(諏訪)(Aug.23-25) Profs. Ruiz-López, Nakata, Abe, Muraoka

For copyright reasons, the images are not displayed.

StudyCamps

SC2018 (Ohmi Hachiman, Shiga)
(近江八幡)(Aug.22-23) Profs. Yu, Watanabe


Himakajima WS (MSCRS20219)
(日間賀島)(Mar.21-22, 2019) Profs. Hirata, Okamoto, Straub, Tanaka, Ota, Koike

SC2019 (Hida Takayama, Gifu)
(飛騨高山)(Sep.1-2, 2019)
Profs. Straub, Lintuluoto, Kitao



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Profs. Straub, Lintuluoto, Kitao

Ncube Competition
Best Presentation Award

StudyCamps

SC2020 (cancelled due to COVID-19)
...

SC2022 (Ohmi Hachiman, Shiga)
(近江八幡)(March 6-7, 2023)
Straub・Bondar・江原・松林・栢沼・大谷・笠原先生

休暇村
おうみはちまん
近江八幡
OHMI HACHIMAN
https://www.qkamura.or.jp/ohmi/

秀吉の甥)が八幡山
開町したことに始まり
と琵琶湖とを繋ぎ、
する船を城下内に寄
で、人・物・情報を集
市楽座制を実施する
大いに活気づけまし
村から車で約20分)

八幡山ロープウェー

水郷地帯が広がるのどかな風景の中に、雄大にそびえる八幡山。標高271mの山頂まではロープウェーで約4分。頂上には、この山に城を築いた豊臣秀次公を祀る村雲御所瑞龍寺があります。
〈休暇村から車で約20分〉

https://cf.bstatic.com/xdata/images/hotel/max1024x768/407617159.jpg?k=33731a1451dfd646f5cfba3c6d20f148468d3bd337a5f595b4bfdfdfa559f338f&o=

https://travel.rakuten.co.jp/HOTEL/76886/CUSTOM/GW76886160210144427.html

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98(H10)0700 Assoc. Prof. of GS. of Human Informatics, NU — Change to NU

10 JST*Computational Science and Technology Specific Research and Development Promotion Project: **ACT-JST** "Study on Non-equilibrium and Non-stationary Dynamics of Aggregation Reaction Systems"

*JST: Japan Science and Tech Corporation

Birth of Lab Ncube !

Birth of "Three "Non"s" !!

02(H14)0304 **Int. Conf.** CRN³ (Clarifying Non-equilibrium non-stationarity characteristic of chemical reaction phenomena)

(Grant-in-aid: C)

02(H14)09 Prof. (Human Info)

03(H15)0405 Prof. (Info. Sci.)

04(H16)0406 21st Century COE "Computational Science Frontiers"

AD

06(H18)1008 JST*Core Research for Evolutionary Science and Technology: **CREST** "Research Development of Multiscale Simulation of Aggregation Reaction Systems"

07(H19)0409 Minor ailment

08(H20)1210

12(H24)0515

13(H25)1016

PACIFICHEM 2015

14(H26)0417

15(H27)12 PACIFICHEM2015

16(H28)0419 MSCRS2016 (JSPS Japan-Brazil+NU)

17(H29)04

Dr. Kurisaki

Ms. Kobayashi

Ms. Fukuhara

18(H30)09

20(R02)12

23(R05)0325 StudyCamp2022

JSPS-FAPESP International Symposium MSCRS2016

"Multi-scale Simulation of Condensed-phase Reacting Systems"

(2016年10月10-13日, AD18)

Noyori Conference Hall

JAPAN SOCIETY FOR THE PROMOTION OF SCIENCE 日本学術振興会

FAPESP SÃO PAULO RESEARCH FOUNDATION

名古屋大学 NAGOYA UNIVERSITY

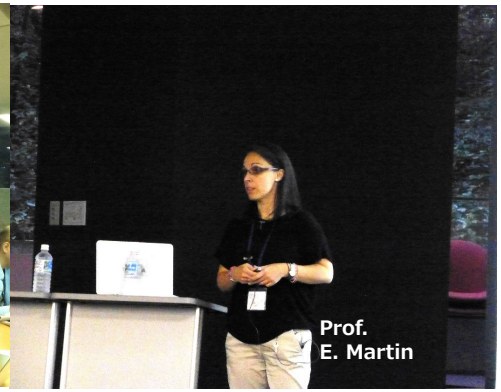
INFORMATION SCIENCE NAGOYA UNIVERSITY

Toast by Dr. Eisuke Kita, Vice-Dean of the Graduate School

JSPS-FAPESP International Symposium MSCRS2016

"Multi-scale Simulation of Condensed-phase Reacting Systems"

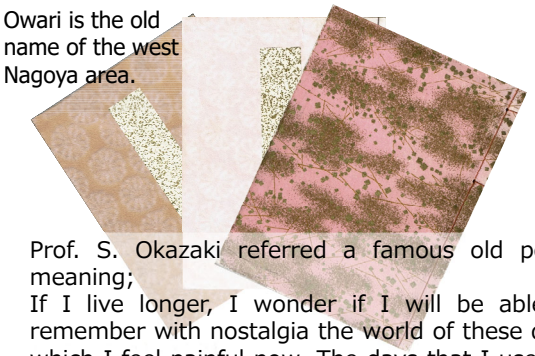
(2016年10月10-13日, AD18)



Owari Complex Seminar & Visitors' Books

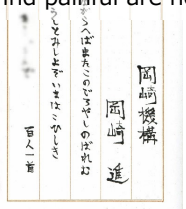
Complex … Complex systems, Complex (chemistry), assembly, gathering place

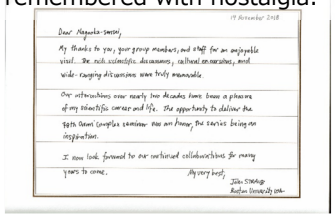
Owari is the old name of the west Nagoya area.

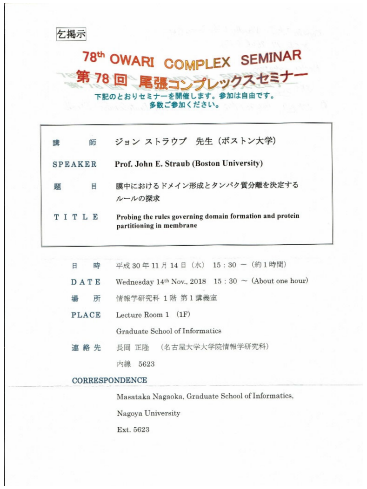


・The Owari Complex Seminar, which started immediately after the move, has been held 79 times!!

Prof. S. Okazaki referred a famous old poem meaning;
If I live longer, I wonder if I will be able to remember with nostalgia the world of these days, which I feel painful now. The days that I used to find painful are now remembered with nostalgia.







15th “Complex Systems Science” Seminar

A seminar series of the division of complex systems science

(’23, AD25)

第15回複雑系科学セミナーのご案内 受信トレイ ×

Ryotaro Koike <rkoike@i.nagoya-u.ac.jp>
To 複雑系科学専攻, students

複雑系科学専攻の先生方・大学院生・研究員の皆様

生命情報論講座の小池です.

第15回複雑系科学セミナーを以下の通り開催します.
お忙しいこととは存じますが，ぜひご参加いただければと思います.

＝＝＝＝＝＝＝＝＝＝＝＝＝＝＝＝＝＝
日時：２０２３年９月２２日（金）　１７時半から１時間程度
（終了後に懇親会開催予定）
場所：情報学研究科棟１Ｆ　第１講義室
講師：生命情報論講座　教授　山西芳裕

タイトル：
人工知能とビッグデータで新薬をつくる

アブストラクト：
近年の生命医科学では、疾患に関するゲノム情報や臨床情報、生体分子に関するオミックス情報、膨大な化合物に関する生物活性情報などが得られるようになった。このようなビッグデータ時代において、人工知能・機械学習の重要性が高まってきており、データ解析から創薬や医療に繋げる役割が求められている。医薬データは、グラフ構造、木構造、文字列、テンソルなど様々なデータ構造を取り、情報科学的にも挑戦的な課題が多い。本セミナーでは、疾患、遺伝子、タンパク質、化合物に関する多様なビッグデータを融合解析し、創薬や医療における様々な課題を解決するための機械学習アルゴリズムの研究を紹介する。創薬標的探索、化合物スクリーニング、シナジー創薬学、細胞直接変換、医薬品分子構造設計などへの応用例をいくつか紹介する。
＝＝＝＝＝＝＝＝＝＝＝＝＝＝＝＝＝＝

Prof. Motonori Ota

Prof. Yoshihiro Yamanishi

Prof. Eisuke Kita, Dean

Ncube Nagaoka Laboratory

Outline

JOURNEY “DEPARTURE”

For copyright reasons, the images are not displayed.

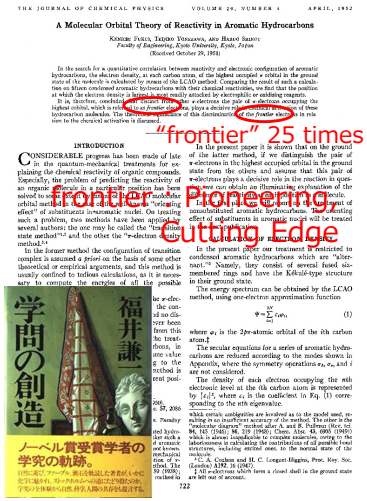
Ncube Nagaoka Laboratory

:01

§5 Concluding Remarks ~Are we carrying on the spirit of Fukui’s lab?~

Attitude of studying in the opposite direction

Value the fundamentals, and strive to learn widely



Kosei Publishing

”To study hard together a subject that does not seem to be related to the path you are trying to follow, or, more extremely, to study in the opposite direction. …“

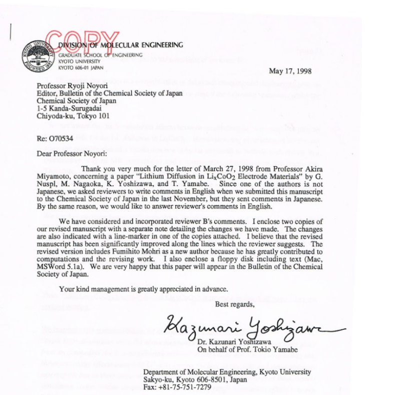
”We never know when or in what form what we have learned will be useful. If we compare learning to a plant, the underground stems of individual studies are connected to each other in unexpected ways.“

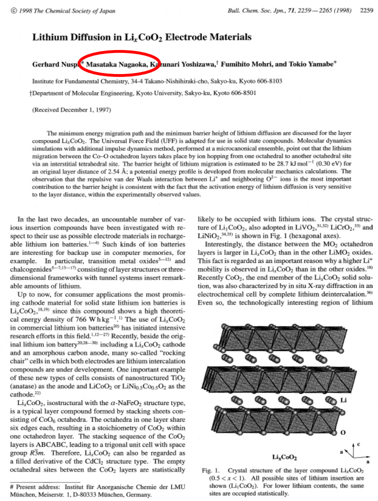
“Students today have too much to learn compared to my time. Given this, one might argue against such idealism. But, knowing this, I would like to emphasize. To be creative, narrow study is not beneficial. We must study broadly at all costs.“ （「The Creation of “Study”」(1984))

In connection with the naming of the frontier orbital theory, he wrote in his book that he studied quantum mechanics, which was the most advanced basic science at that time, and wondered if he could apply it.

Co-authored paper with Dr. Yoshizawa (1998)

"Lithium Diffusion in Li_xCoO_2 Electrode Materials"





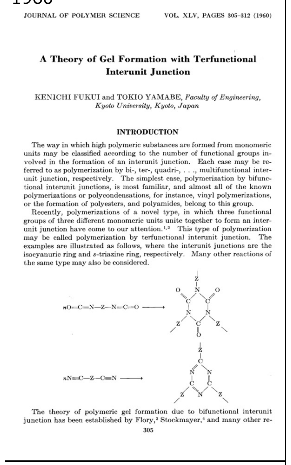
Prof. Yamabe's Doctoral Thesis (1967)

「Study on gelation by bonding between multifunctional grouping unit」

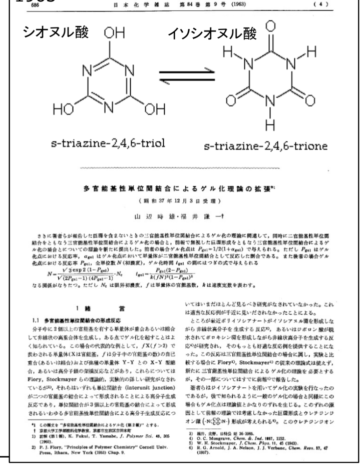
1964

"I (Dr. Yamabe) was assigned to the laboratory of Prof. Fukui as a graduation research student in April 1958, with the intention of studying **quantum chemistry**, but for some reason I was assigned to be directly supervised by Prof. Fukui for the time being. The subject was not quantum chemistry, but a "**theoretical study on the gelation phenomenon of polymers with a special isocyanurate (isocyanurate ring) bonding mode,**" which had nothing to do with the other members, and Prof. Fukui asked me to develop from statistical mechanics what he had already been working on from kinetics." (「Rakuho(洛朋)19」(2010))

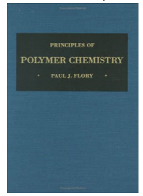
1960



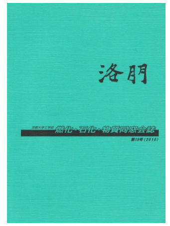
1963



Cornell University Press



P. J. Flory
「Polymer Chemistry」
(1953)



「Rakuho(洛朋)19」
(2010)

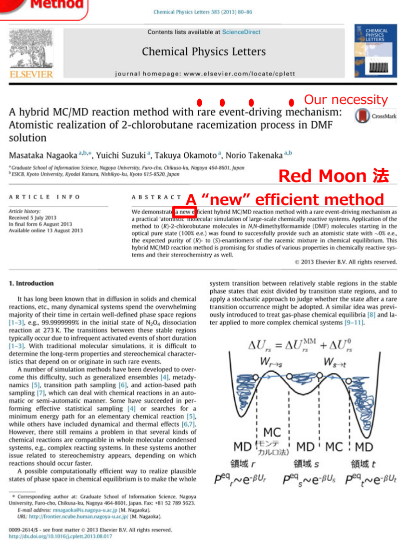
第８章　線状高分子の分子量分布
　　　　二官能基性単位間結合
第９章　非線状高分子の分子量分布とゲル化理論
　　　　三官能基性枝分れ高分子

拡張１：　巨環＊なしの三官能基性単位間結合
拡張２：　(拡張１)＋二官能基性単位間結合
拡張３：　巨環ありの三官能基性単位間結合
＊巨環（macroring）

Establishment of Computational Molecular Technology towards Macroscopic Chemical Phenomena

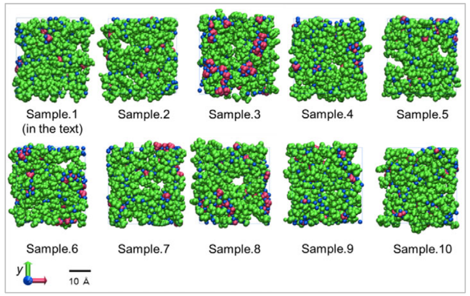
~Complex chemical reactions, stereospecificity, aggregate structure~

RM Method



When,
6 years old　62 years old!

When,
12 years old　67 years old!



Ncube
Nagaoka Laboratory

"Backpropagation Method"

- A method for efficiently computing the derivative of the evaluation function -

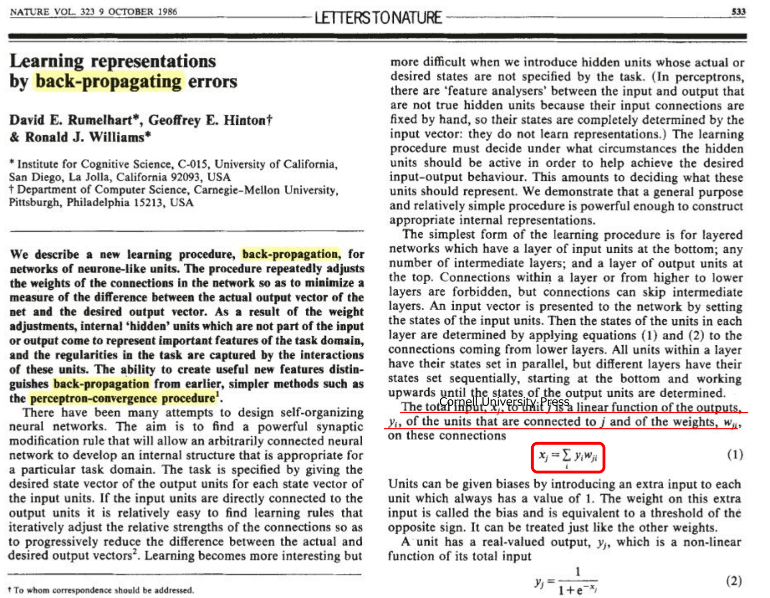
Image credit:L.A. Cicero

D.E. Rumelhart
(1942-2011)

G.E. Hinton
(1947-　)

Image credit:
Linda Nylind / eyevine via Redux

H.C. Longuet-Higgins
(1923-2004)
Cambridge U.('54-'67)
Edinburgh U.('67-'74)



・D.E. Rumelhart, G.E. Hinton, R.J. Williams, *Nature*, 323, 533 (1986)

A little further, while learning the fundamentals carefully and extensively !

RM Method

Chemical Physics Letters

A hybrid MC/MD reaction method with rare event-driving mechanism: Atomistic realization of 2-chlorobutane racemization process in DMF solution

Our necessity

Red Moon 法

A "new" efficient method

When,
6 years old 62 years old!

years old 67 years old

©写真AC

Ncube changed the mode for the time being!
Thank you very much for your long-time support!







Collaborators and Students:

・N.O.-Yoshida（DR）・I.Okazaki（DR）・Y.Hara（DR）
・T.Okamoto（PD）・M.Takayanagi（PD）・Y.Koyano（PD）
・Y.Oishi（M2）・N.Yamamoto（DR）・K.Yamada (DR)
・I.Kurisaki（DR）・N.Takenaka（DR）・Y.Suzuki（DR）
・Y.Kitamura（DR）・K.Matsumoto（DR）
(Other OBs & OGs and outer Coworkers)

新機能創出を目指した分子技術の構築
Establishment of Molecular Technology towards the Creation of New Functions

Gaussian Interface for AMBER9

住友化学
DAICEL
三井化学
AsahiKASEI
ShinEtsu
ENEOS
富士電機

Ncube Nagaoka Laboratory

Thank you for your attention!

**Graduates, Postdoc fellows,
Collaborators, Lab staffs, it was
a pleasure working with all of you!
I appreciate your continued support!**