

## 研究業績リスト

吉森 明

1. 学位論文: 電子移動反応におけるエネルギーギャップ則の理論的研究  
(理学博士、名古屋大学、1991年3月)

### 2. 原著論文

主要論文は をつけて太字にした。また、学生を指導した研究については「学生指導」と書いた。

- [1] Transfer Coefficient in Electrochemical Reactions,  
A. Yoshimori, T. Kakitani and N. Mataga,  
J. Phys. Chem., 1989, Vol. 93, No. 9, 3694-3702.
- [2] **Shapes of the Electron-Transfer Rate vs Energy Gap Relations in Polar Solutions,**  
**A. Yoshimori, T. Kakitani, Y. Enomoto and N. Mataga,**  
**J. Phys. Chem., 1989, Vol. 93, No. 26, 8316-8323.**
- [3] Theoretical Study of Dielectric Saturation in Molecular Solutions by the Monte Carlo Simulation,  
Y. Hatano, T. Kakitani, A. Yoshimori, M. Saito and N. Mataga,  
J. Phys. Soc. Japan, 1990, Vol. 59, No. 3, 1104-1116.
- [4] Theoretical Study of the Free Energy Curve as a Function of Reaction Coordinate of Electron Transfer by the Cumulant Expansion Method,  
A. Yoshimori and T. Kakitani,  
J. Chem. Phys., 1990, Vol. 93, No. 7, 5140-5146.
- [5] Monte Carlo Simulation Study of Free Energy Curves for Electron Transfer Reactions in Polar Solutions by Considering the Electronic Polarizability,  
Y. Hatano, T. Kakitani, Y. Enomoto and A. Yoshimori,  
Mol. Simu., 1991, Vol. 6, 191-198.
- [6] Monte Carlo Simulation Study on Reorganization Energy of Electron-Transfer Reactions in Polar Solution,  
Y. Enomoto, T. Kakitani, A. Yoshimori, Y. Hatano and M. Saito,  
Chem. Phys. Letters, 1991, Vol. 178, No. 2,3, 235-240.
- [7] Non-Linear Effects on Solvation Dynamics,  
A. Yoshimori,

- Chem. Phys. Letters, 1991, Vol. 184, No. 1,2,3, 76-80.
- [8] Monte Carlo Simulation Study on Energy-Gap Dependence of Electron-Transfer Reactions in Polar Solution: Effect of Electronic Polarizability of Solvent, Y. Enomoto, T. Kakitani, A. Yoshimori and Y. Hatano, Chem. Phys. Letters, 1991, Vol. 186, No. 4,5, 366-371.
- [9] Energy Gap Dependence of the Solvent Dynamics Effect on Electron Transfer Rates in Non-Linear Response Systems, A. Yoshimori and T. Kakitani, J. Phys. Soc. Japan, 1992, Vol. 61, No. 7, 2577-2592.
- [10] Effects of the Donor-Acceptor Distance Distribution on the Energy Gap Laws of Charge Separation and Charge Recombination Reactions in Polar Solutions, T. Kakitani, A. Yoshimori and N. Mataga, J. Phys. Chem., 1992, Vol. 96, No. 13, 5385-5392.
- [11] Rossby Number Dependence on Meander Dynamics of a Potential Vorticity Front, A. Yoshimori, J. Oceanogr., 1993, Vol. 49, No. 5, 521-533.
- [12] Horizontal Divergence Caused by Meanders of a Thin Jet, A. Yoshimori, J. Phys. Oceanogr., 1994, Vol. 24, No. 2, 345-352.
- [13] Effects of Interaction between Two Warm-Core Rings on Phytoplankton Distribution, A. Yoshimori and M. J. Kishi, Deep-Sea Res., 1994, Vol. 41, No. 7, 1039-1052.
- [14] Symmetry of a Free Energy Curve in Polar Solution, A. Yoshimori, Chem. Phys. Letters, 1994, Vol. 225, 494-498.
- [15] Nonlinear Quantum Effects on Electron Transfer Reactions, A. Yoshimori, Chem. Phys. Letters, 1995, Vol. 235, 303-308.
- [16] Modeling of Spring Bloom in the Western Subarctic Pacific (off Japan) with Observed Vertical Density Structure, A. Yoshimori, J. Ishizaka, T. Kono, H. Kasai, H. Saito, M. J. Kishi and S. Taguchi,

- J. Oceanogr., 1995, Vol. 51, 471-488.
- [17] Present and Future Perspectives of Theoretical Aspects of Photoinduced Charge Separation and Charge Recombination Reactions in Solution,  
T. Kakitani, N. Matsuda, A. Yoshimori and N. Mataga,  
Prog. Reaction Kinetics, 1995, Vol. 20, 347-381.
- [18] Effects of Diffusion on Geminate Charge Recombination,  
A. Yoshimori, K. Watanabe, and T. Kakitani,  
Chem. Phys., 1995, Vol. 201, 35-46.
- [19] Nonlinear Effects of Solvation Dynamics,  
A. Yoshimori,  
J. Mol. Liquid, 1995, Vol. 65/66, 297-300.
- [20] Refraction of Active Waves in Reaction-Diffusion Media,  
H. Yamada, C. Matuoka, and A. Yoshimori,  
Phys. Lett. A, 1996, Vol. 210, 189-194.
- [21] Nonlinear terms due to many-particle correlation in the density functional theory  
A. Yoshimori  
J. Chem. Phys., 1996, Vol. 104, 9586-9592.
- [22] Analysis of the Temperature Dependence of Femtosecond Excited State Dynamics of Bacteriorhodopsin by Spin-Boson Model,  
R. Akiyama, A. Yoshimori, T. Kakitani, Y. Imamoto, Y. Shichida and Y. Hatano,  
Chem. Phys. Letters, 1996, Vol. 256, 165-171. 学生指導
- [23] Nonlinear Effects of Number Density for Solvent Molecules on Solvation Dynamics,  
A. Yoshimori,  
J. Chem. Phys., 1996, Vol. 105, 5971.
- [24] Analysis of the Excited-State Dynamics of 13-trans-locked-Bacteriorhodopsin,  
R. Akiyama, A. Yoshimori, T. Kakitani, Y. Imamoto, Y. Shichida, and Y. Hatano,  
J. Phys. Chem. A, 1997, Vol 101, 412-417. 学生指導
- [25] Monte Carlo Simulation Study on the Structure and Reaction at Metal-Electrolyte Interface,  
N. Goto, A. Okada, T. Kakitani, A. Yoshimori, and Y. Hatano,  
J. Phys. Soc. of Japan, 1997, Vol 66, 1825-1835. 学生指導
- [26] Variability in timing and magnitude of spring bloom in the Oyashio region, the

- western subarctic Pacific off Hokkaido, Japan,  
H. Kasai, H. Saito, A. Yoshimori, and T. Taguchi,  
Fish. Oceano., 1997, Vol. 6, 118-129.
- [27] Nonlinear Quantum Effects on Electron Transfer Reactions,  
Akira Yoshimori,  
Journal of Electroanalytical Chemistry, 1997, Vol. 438, 21-26.
- [28] **An Investigation of Dynamical Density Functional Theory for Solvation in Simple Mixtures,**  
**Akira Yoshimori, T.J.F.Day, and G.N.Patey**  
**Journal of Chemical Physics, 1998 Vol. 108, 6378.**
- [29] Theory of Ion Solvation Dynamics in Mixed Dipolar Solvents,  
Akira Yoshimori, T.J.F.Day, and G.N.Patey,  
Journal of Chemical Physics, 1998, Vol. 109 3222.
- [30] Mathematical models of population dynamics of the kelp (*Laminaria religiosa*)  
with emphasis on temperature dependence,  
Akira Yoshimori, Tokihiro Kono and Hitoshi Iizumi,  
Fisheries Oceanography, 1998, Vol. 7, No. 2, 136.
- [31] Comparisons of semiclassical approximations by expansion in Planck's constant,  
Akira Yoshimori,  
Journal of Chemical Physics, 1998 Volume 109, Issue 20, 8790-8800.
- [32] Derivation of Kuramoto-Sivashinsky equation by the renormalization group  
method,  
Tsuyoshi Maruo, Kazuhiro Nozaki and Akira Yosimori,  
Prog. Theor. Phys, 1999 Vol. 101, No. 2, 243.
- [33] Nonlinear Langevin equations and the time dependent density functional method,  
Akira Yoshimori,  
Phys. Rev. E, 1999, Vol. 59, 6535.
- [34] Microscopic derivation of jump rate distribution and the glass transition,  
T Odagaki and A Yoshimori,  
Journal of Physics: Condens. Matter, 2000, Vol. 12, 6509-6514.
- [35] Localization transition in vitrification process,  
T Odagaki and A Yoshimori,  
Physica B 296 (2001) 174-179.
- [36] A Time Dependent Density Functional Method for the Interaction Site Model,

- Akira Yoshimori,  
Journal of Molecular Liquids, 2001, Vol. 90 29-33.
- [37] Nonlinear Distribution Dynamics of Solvation,  
Akira Yoshimori  
Journal of the Physical Society of Japan, 2001, Vol 70 No. 6 1833-1841.
- [38] Specific heat in nonequilibrium systems,  
Toshiaki Tao, Akira Yoshimori, and Takashi Odagaki  
Phys. Rev. E, 2001, Vol. 64, 046112. 学生指導
- [39] Spatial Mosaic and Interfacial Dynamics in a Müllerian Mimicry System,  
Akira Sasaki, Isao Kawaguchi, Akira Yoshimori,  
Theoretical Population Biology, 2002, Vol. 61, No. 1, 49-71.
- [40] Specific heat in a nonequilibrium system composed of Einstein oscillators,  
Toshiaki Tao, Akira Yoshimori, and Takashi Odagaki,  
Phys. Rev. E, 2002, Vol. 66, 041103. 学生指導
- [41] Specific heat of nonequilibrium systems and glass transition,  
Takashi Odagaki, Toshiaki Tao, and Akira Yoshimori  
Journal of Non-Crystalline Solids, 2002, Vol. 307-310, 407-411.
- [42] Specific heat anomaly at the glass transition,  
Takashi Odagaki, Takashi Yoshidome, Toshiaki Tao, and Akira Yoshimori,  
Journal of Chemical Physics, 2002, Vol. 117, 10151-10155. 学生指導
- [43] Selective solvation caused by size effects,  
Masashi Sakurai and Akira Yoshimori,  
Chemical Physics Letters, 2003, Vol. 371, 23–28. 学生指導
- [44] Time dependent density functional methods and their application to chemical physics,  
Akira Yoshimori,  
Theoretical and Computational Chemistry 2004, Vol. 3, No. 1, 117-144.
- [45] Cooling rate dependence of specific heat in systems out of equilibrium  
T. Tao, T. Odagaki, and A. Yoshimori  
Journal of Chemical Physics, 122, 044505 (2005). 学生指導
- [46] **Microscopic derivation of time-dependent density functional methods,**  
**Akira Yoshimori,**  
**Physical Review E 71, 031203 2005.**

- [47] A microscopic model of jump rate distribution in the glass transition,  
Akira Yoshimori, Takashi Odagaki,  
*J. Phys. Soc. Jpn.*, Vol.74, No.4, p.1206-1213, 2005
- [48] Bandwidth analysis of solvation dynamics in a simple liquid mixture,  
M. Sakurai and A. Yoshimori,  
*J. Chem. Phys.* **122**, 104509 (2005) (7 pages). 学生指導
- [49] Free energy landscape approach to glass transition,  
T. Odagaki, T. Yoshidome, A. Koyama, and Akira Yoshimori  
*Journal of Non-Crystalline Solids*, **352**, 4843-4846 (2006). 学生指導
- [50] Construction of the free energy landscape by the density functional approach,  
Takashi Yoshidome, Akira Yoshimori and Takashi Odagaki  
*Journal of the Physical Society of Japan*, **Vol.75**, No.5, 054005, 2006 (4 pages).  
学生指導
- [51] Nonlinear effects on solvation dynamics in simple mixtures,  
Shuhei Murata and Akira Yoshimori  
*The Journal of Chemical Physics*, **Vol. 125**, 244501 (2006) (8 pages). 学生指導
- [52] **Free energy landscape and cooperatively rearranging region in a hard sphere glass,**  
**Takashi Yoshidome, Akira Yoshimori, and Takashi Odagaki**  
*Physical Review E* **76**, 021506 (2007) (7 pages). 学生指導
- [53] A molecular theory of large-solute diffusion,  
Akira Yoshimori  
*Condensed Matter Physics*, **10**, 563, (2007).
- [54] New conditions for validity of the centroid molecular dynamics and ring polymer molecular dynamics,  
Akira Yoshimori  
*The Journal of Chemical Physics*, **Vol. 128**, 234105 (2008).
- [55] Free energy landscape for a tagged particle in a dense hard sphere liquid,  
T. Yoshidome, T. Odagaki, and Akira Yoshimori,  
*Physical Review E.*, **Vol. 77** 061503 (2008). 学生指導
- [56] Derivation of the nonlinear fluctuating hydrodynamic equation from under-damped Langevin equation,  
T. Nakamura and Akira Yoshimori,  
*Journal of Physics A: Mathematical and Theoretical*, **Vol. 42** 065001 15pp (2009).

- [57] Free Energy Landscape Theory of Glass Transition and Entropy,  
Takashi Odagaki and Akira Yoshimori,  
*Journal of Non-Crystalline Solids*, **Vol. 355** 681 (2009).
- [58] Studies of liquid-solid transitions using a thermodynamic perturbation method  
with modified weighted density approximation,  
Ayumi Suematsu, Akira Yoshimori, Takashi Odagaki,  
*Journal of the Physical Society of Japan*, **Vol. 80** 025001 (2011). 学生指導
- [59] Time Dependent Density Functional Theory Formulated by the Interaction-Site  
model,  
Akira Yoshimori  
*Journal of the Physical Society of Japan*, **Vol. 80** 034801 (2011).
- [60] Configurational Entropy and Heat Capacity in Supercooled Liquids,  
Akira Yoshimori and Takashi Odagaki  
*Journal of the Physical Society of Japan*, **Vol. 80** 064601 (2011).
- [61] A Theory of Hole Transfer in DNA,  
Takaki Himeno, Akira Yoshimori,  
*Journal of the Physical Society of Japan*, **Vol. 81** 093801 (2012). 学生指導
- [62] New macroscopic expression connecting energy dissipation with violation of fluctuation  
response relation in colloidal many-particle systems,  
Akira Yoshimori and Takahiro Harada  
*Journal of the Physical Society of Japan*, **Vol. 81** 094002 (2012).
- [63] **Perturbation theory of large-particle diffusion,**  
**Yuko Inayoshi, Akira Yoshimori, and Ryo Akiyama**  
*Journal of the Physical Society of Japan*, **Vol. 81** 114603 (10 pages)  
(2012). 学生指導
- [64] Molecular dynamics study of fast dielectric relaxation of water around a  
molecular-sized ion,  
Yoji Kubota, Akira Yoshimori, Nobuyuki Matubayasi, Makoto Suzuki, and Ryo  
Akiyama  
*The Journal of Chemical Physics*, **Vol. 137**, 224502 (2012).
- [65] A Time Dependent Density Functional Theory of Polarization Relaxation under  
External fields,  
Y. Uematsu, and A. Yoshimori  
*Journal of the Physical Society of Japan*, **Vol. 82** 013001 (4 pages) (2013). 学生

## 指導

- [66] A theoretical framework for calculations of the structural relaxation time on the basis of the free energy landscape theory,  
Toru Ekimoto, and A. Yoshimori, Takashi Odagaki, and Takashi Yoshidome  
*Chemical Physics letter*, **Vol. 577**, 58 (2013). 学生指導
- [67] Perturbation Theory of Large-Particle Diffusion in a Binary Solvent Mixture,  
Yuka Nakamura, Akira Yoshimori, and Ryo Akiyama  
*Journal of the Physical Society of Japan*, **Vol. 83**, 064601 (2014). 学生指導
- [68] A Unified Proof of the Harada-Sasa equality for Underdamped and Overdamped Systems,  
Kazuo Yamada and Akira Yoshimori  
*Journal of the Physical Society of Japan*, **Vol. 83**, 053001 (2014). 学生指導
- [69] Solid phase stability of a double-minimum interaction potential system,  
Ayumi Suematsu, Akira Yoshimori, Masafumi Saiki, Jun Matsui and Takashi Odagaki  
*The Journal of Chemical Physics*, **Vol. 140**, 244501 (2014). 学生指導
- [70] Shankar P. Das<sup>1</sup>, and Akira Yoshimori Coarse-grained forms for equations describing the microscopic motion of particles in a fluid,, *Phys. Rev. E* 88, 043008 (2013) [8 pages]
- [71] A Theory of Solvation Effects on Viscosity,  
Tomofumi Yamakita and Akira Yoshimori  
*Journal of the Physical Society of Japan*, **Vol. 84**, 043602 (2015). 学生指導
- [72] A Unified Expression of Harada-Sasa Equality in Underdamped and Overdamped Langevin Systems of the Field Variable Description,  
Kazuo Yamada and Akira Yoshimori  
*Journal of the Physical Society of Japan*, **Vol. 84**, 044008 (2015). 学生指導

## 3. 国際会議プロシーディングス

すべて査読付きです。

1. Theoretical Analysis of Energy Gap Laws of Electron Transfer Reactions by Considering the Distribution of the Donor and Acceptor Distance,  
T. Kakitani, [Akira Yoshimori](#) and N. Mataga,  
In *Electron Transfer in Inorganic, Organic, and Biological Systems, Advances*



- in Chemistry Series*, J. Bolton, N. Mataga and G. McLendon, editors, American Chemical Soc., 1991, Chap. 4, p. 46-69.
2. Free energy landscape and CRR of glass-forming substance,  
Takashi Yoshidome, Akira Yoshimori and Takashi Odagaki  
Flow Dynamics: The second international conference on flow dynamics, edited  
by M. Tokuyama and S. Maruyama, *AIP Conference Proceedings* **832**, 188-191  
(2006). 学生指導
  3. Separation of Dynamics in the Free Energy Landscape,  
Toru Ekimoto, Takashi Odagaki and Akira Yoshimori  
CP982, Complex Systems, eds. M. Tokuyama, I. Oppenheim and H. Nishiyama,  
(AIP, 2008) 211-214. 学生指導
  4. Application of Phase Transition Theory to Glass Transition System,  
Ayumi Suematsu, Akira Yoshimori, Masafumi Saiki, Jun Matsui, and Takashi  
Odagaki  
*Journal of the Physical Society of Japan*, **Vol. 81** Supplement A SA020 (7  
pages) (2012). 学生指導
  5. A Perturbation Theory for Friction of a Large Particle Immersed in a Binary  
Solvent,  
Yuka Nakamura, Akira Yoshimori, and Ryo Akiyama,  
*Journal of the Physical Society of Japan*, **Vol. 81** Supplement A SA026 (7  
pages) (2012). 学生指導
  6. Application of Phase Transition Theory to Glass Transition System,  
Ayumi Suematsu, Akira Yoshimori, Masafumi Saiki, Jun Matsui, and Takashi  
Odagaki  
*Journal of the Physical Society of Japan*, **Vol. 81** Supplement A SA020 (7  
pages) (2012). 学生指導
  7. Effects of the Solvation Structure on Diffusion of a Large Particle in a Binary  
Mixture Studied by Perturbation Theory,  
Yuka Nakamura, Akira Yoshimori, and Ryo Akiyama  
*Journal of Molecular Liquids*, **Vol. 81** Supplement A SA026 (7 pages) (2012).  
学生指導
  8. A non-perturbative approach to freezing of superfluid  $^4\text{He}$  in density functional  
theory,  
T. Minoguchi<sup>1</sup>, D.E. Galli, M. Rossi and Akira Yoshimori,

- Journal of Physics: Conference Series, 400, 012050, (2013)
9. Journal of Molecular Liquids, Volume 200, Part A, December 2014, Pages 85-88,  
Effects of the solvation structure on diffusion of a large particle in a binary mixture studied by perturbation theory,  
Y.Nakamura, A.Yoshimori, R.Akiyama. 学生指導
  10. Volume 200, Part A, December 2014, Pages 81-84 Journal of Molecular Liquids  
Effects of interactions between particles on dynamics in microrheology Masao Inoue and Akira Yoshimori. 学生指導
  11. A. Suematsu, A. Yoshimori, M. Saiki, J. Matsui, T. Odagaki Control of solid-phase stability by interaction potential with two minima, Journal of Molecular Liquids, Volume 200, Part A, Pages 12-15 (2014). 学生指導

#### 4. 著書

1. 吉森明、  
日本光合成研究会編 “光合成事典”2 項目執筆、2003

#### 5. 総説・解説

1. ガラスと自由エネルギー、  
吉森明  
物性研究 84-1 (2005-4) 59-78.
2. Yamaguchi theory and Van der Waals picture  
吉森明、稲吉裕子、秋山良  
物性研究 91 (2009) 713.

#### 6. 招待講演

##### (1) 国際会議

1. “Nonlinear dynamics of molecular liquids”  
1999年7月、26th International Conference on Solution Chemistry、Fukuoka,  
Japan  
Akira Yoshimori
2. “Free energy landscape and glass transition”

- 2007年11月、Fukuoka International Workshop on Unifying Concepts of Glass Transition, Kyushu University  
A. Yoshimori, T. Odagaki, T. Yoshidome and T. Ekimoto
3. “Free energy landscape and configurational entropy”  
2008年11月、Unifying Concepts in Glass Physics IV, Kyoto  
A. Yoshimori and T. Odagaki
4. “Perturbation Theory of Large-Particle Diffusion”  
日韓ワークショップ (16 Dec. 2012, Fukuoka)  
Akira Yoshimori<sup>1</sup>, Yuka Nakamura<sup>1</sup>, Yuko Inayoshi<sup>1</sup>, and Ryo Akiyama
5. “Control of solid phase stability by interaction potential with two minima”  
7th Mini-Symposium on Liquids (2013年7月5日(金) 6日(土))  
Akira Yoshimori, Ayumi Suematsu, Masafumi Saiki, Jun Matsui, and Takashi Odagaki

## (2) 国内会議

1. “海洋混合層モデルと生態系モデル-1-”  
1994年12月、海洋研シンポジウム、東京大学海洋研究所  
吉森明
2. “溶液の動的性質における理論的研究”  
1997年11月、第20回溶液シンポジウム、京都大学化学研究所  
吉森明
3. “溶媒和における非線形応答”  
2000年8月、第10回理論化学シンポジウム、愛知  
吉森明
4. “分子論から見たガラス転移とブラウン運動”  
2001年5月、分子研研究会、分子科学研究所  
吉森明
5. “構造ガラスにおける自由エネルギーランドスケープとは何か?”  
2004年8月、東京大学物性研究所短期研究会「極端非平衡系の物性とエネルギーランドスケープ」、物性研  
吉森明
6. “溶液化学と非平衡物理”  
2011年11月、溶液化学シンポジウム、名古屋大学

吉森明

7. “液体における非平衡現象の理論”

2012年2月18日、重イオン衝突と非平衡物理の理論的発展、理化学研究所

吉森明

(3) その他の招待講演

依頼講演、招待されたセミナーを含みます。ただし、自主的に講演したセミナーは除いてあります。

1. “溶媒和ダイナミックスの理論”

1994年11月、科件費総合研究(B)研究会、名古屋

吉森明

2. “溶媒和ダイナミックスにおける非線形の効果”

1995年2月、物理化学セミナー、京都大学

吉森明

3. “溶媒和ダイナミックスの理論的研究”

1996年1月、金沢大学

吉森明

4. “Dynamics of distribution in solvation ”

1999年11月4日、COE プロジェクト「光反応機構・光反応制御」セミナー、通産省物質研究所

吉森明

5. “溶液のダイナミックスにおける非線形効果”

1999年11月13日、大阪大学 VBL 若手研究会、大阪大学

吉森明

6. “溶媒のダイナミックスと化学反応の理論”

2001年8月、「理論分子科学の最先端」(科学研究費特定領域研究)、慶應義塾大学

吉森明

7. “動的溶液理論入門”

2003年8月、2003年液体夏の学校講師、京都

吉森明

8. “液体のダイナミックスと非平衡物理学”

2003年9月、名古屋大学情報学科学研究科集中講義、名古屋

吉森明

9. “ガラスと自由エネルギー”

2004年12月、非線形数理冬の学校、東京

吉森明

10. “非平衡物理と分子科学”

2005年8月、分子科学若手の会 夏の学校 2005、滋賀

吉森明

11. “セントロイド分子動力学 (CMD) 法の基礎付けについて”

2005年9月、分子科学研究所

吉森明

12. “Yamaguchi theory and Van der Waals picture”

2008年11月、2nd Mini-Symposium on Liquids, 九州大学

吉森明、稲吉裕子、秋山良

7. 受賞

特になし