

研究発表

(1) 学会誌等

1. 量子化学基礎理論の精密化と再構築

1. H. Nakatsuji, "Structure of the Exact Wave Function. IV. Excited States from Exponential Ansatz and Comparative Calculations by the Iterative Configuration Interaction and Extended Coupled Cluster Theories", J. Chem. Phys., 116, 1811-1824 (2002).

2. H. Nakatsuji, "Inverse Schrödinger Equation and the Exact Wave Function", Phys. Rev. A 65, 052122-1-15 (2002).

3. H. Nakatsuji and M. Ehara, "Structure of the Exact Wave Function. V. Iterative Configuration Interaction Method for Molecular Systems within Finite Basis", J. Chem. Phys., 117, 9-12 (2002).

4. M. Nakata, M. Ehara, and H. Nakatsuji, "Density Matrix Variational Theory: Application to the Potential Energy Surfaces and Strongly Correlated Systems", J. Chem. Phys., 116, 5432-5439 (2002).

5. M. Nakata, M. Ehara and H. Nakatsuji, "Density Matrix Variational Theory: Strength of Weinhold-Wilson Inequalities", Fund. World. Quat. Chem., I, 543-557 (2003).

6. H. Nakatsuji, "Scaled Schrödinger Equation and the Exact Wave Function", Phys. Rev. Lett. 93, 030403-1-4 (2004).

7. H. Nakatsuji and M. Ehara, "Iterative CI general singles and doubles (ICIGSD) method for calculating the exact wave functions of the ground and excited states of molecules", J Chem. Phys, 122, 194108 1-7 (2005).

8. H. Nakatsuji and H. Nakashima, "Analytically Solving Relativistic Dirac-Coulomb Equation for Atoms and Molecules", Phys. Rev. Lett., 95, 050407 (2005).

9. H. Nakatsuji, "General Method of Analytically Solving the Schrödinger Equation of Atoms and Molecules", Phys. Rev. A, in press.

10. Y. Kurokawa, H. Nakashima, and H. Nakatsuji, "Free ICI (Iterative Complements Interaction) Calculations of Hydrogen Molecule", Phys. Rev. A, in press.

2. ファインなスペクトロスコピーと反応の量子ダイナミックス

1. Y. Honda, M. Hada, M. Ehara and H. Nakatsuji, "Excited and Ionized States of p-Benzoquinone and Its Anion Radical: SAC-CI Theoretical Study", *J. Phys. Chem. A.*, 106, 3838-3849 (2002).
2. A.K. Das, M. Ehara, H. Nakatsuji, "Excited States of Na and Al Iso-Electronic Ions: SAC-CI Study", *Intern. J. Quantum Chem.*, 87, 81-88 (2002).
3. K. Ishimua, M. Hada, and H. Nakatsuji, "Ionized and Excited States of Ferrocene: Symmetry Adapted Cluster - Configuration Interaction Study", *J. Chem. Phys.*, 117, 6533-6537 (2002).
4. K. Toyota, M. Ehara, H. Nakatsuji, "Elimination of Singularities in Molecular Orbital Derivatives: Minimum Orbital-Deformation (MOD) Method", *Chem. Phys. Lett.*, 356, 1-6 (2002).
5. M. Ehara, M. Ishida, and H. Nakatsuji, "Fine Theoretical Spectroscopy Using SAC-CI General-R Method: Outer- and Inner-Valence Ionization Spectra of CS₂ and OCS", *J. Chem. Phys.*, 117, 3248-3255 (2002).
6. Y. Honda, M. Hada, M. Ehara, and H. Nakatsuji, "Excited and Ionized States of Aniline: SAC-CI Theoretical Study", *J. Chem. Phys.*, 117, 2045-2052 (2002).
7. P. Tomasello, M. Ehara and H. Nakatsuji, "Electronic Excitation Spectra of Cl₂O, ClOCl, and F₂O: A SAC-CI Study", *J. Chem. Phys.*, 116, 2425-2432 (2002).
8. M. Ishida, M. Ehara, and H. Nakatsuji, "Outer- and Inner-Valence Ionization Spectra of NH₃, PH₃, and AsH₃: SAC-CI General-R Study", *J. Chem. Phys.*, 116, 1934-1943 (2002).
9. Y. Honda, M. Hada, M. Ehara, H. Nakatsuji, J. Downing, J. Michl, "Relativistic Effects on Magnetic Circular Dichroism Studied by GUHF/SECI Method", *Chem. Phys. Lett.*, 355, 219-225 (2002).
10. T. Yonehara, S. Kato, "Role of isomerization channel in unimolecular dissociation reaction H₂CO→H₂+CO: ab initio global potential energy surface and classical trajectory analysis", *J. Chem. Phys.*, 117, 11131-11138 (2002).
11. M. Tashiro, S. Kato, "Quantum dynamics study on predissociation of H₃ Rydberg states:

Importance of indirect mechanism”, *J. Chem. Phys.*, 117, 2053-2062 (2002).

12. M. Tashiro, S. Kato, “Predissociation of H_3 2s Rydberg state: quantum dynamics study”, *Chem. Phys. Lett.*, 354, 14-19 (2002).

13. M. Ehara, M. Ishida, K. Toyota, H. Nakatsuji, “SAC-CI General-R Method: Theory and Applications to the Multi-Electron Processes”, 293-319 (2003).

14. P. Tomasello, M. Ehara, and H. Nakatsuji, “Theoretical Investigation on the Valence Ionization Spectra of Cl_2O , $ClOOC$, and F_2O by Correlation-Based Configuration Interaction Methods”, *J. Chem. Phys.*, 118, 5811-5820 (2003).

15. M. Ehara, S. Yasuda and H. Nakatsuji, “Fine Theoretical Spectroscopy Using SAC-CI General-R Method: Outer- and Inner-Valence Ionization Spectra of N_2O and HN_3 ”, *Z. Phys. Chem.*, 217, 161-176 (2003).

16. K. Toyota, M. Ishida, M. Ehara, M. J. Frisch, H. Nakatsuji, “Singularity-Free Analytical Energy Gradients for the SAC/SAC-CI Method: Coupled Perturbed Minimum Orbital-Deformation (CPMOD) Approach”, *Chem. Phys. Lett.*, 367, 730-736 (2003).

17. R. Fukuda, M. Hada, and H. Nakatsuji, “Quasirelativistic Theory for the Magnetic Shielding Constant. II. Gauge-Including Atomic Orbitals and Applications to Molecules”, *J. Chem. Phys.*, 118, 1027-1035 (2003).

18. R. Fukuda, M. Hada, and H. Nakatsuji, “Quasirelativistic Theory for the Magnetic Shielding Constant. I. Formulation of Douglas-Kroll-Hess Transformation for the Magnetic Field and Its Application to Atomic Systems”, *J. Chem. Phys.*, 118, 1015-1026 (2003).

19. T. Yamashita, S. Kato, “Regularity in highly excited vibrational dynamics of $NOCl$ (X^1A'): Quantum mechanical calculations on a new potential energy surface”, *J. Chem. Phys.*, 119, 4251-4261 (2003).

20. M. Ishida, K. Toyota and M. Ehara, M.J. Frisch, H. Nakatsuji, “Analytical Energy Gradient of the Symmetry-Adapted-Cluster Configuration-Interaction General-R method for singlet to Septet Ground and Excited States *J. Chem. Phys.*, 120, 2593-2605 (2004).

21. R. Fukuda, M. Hada, and H. Nakatsuji, "Generalized-UHF Theory for Magnetic Properties with Quasi-Relativistic Hamiltonian", *Rec. Adv. Comp. Chem.* 5, 191-220, (2004).
22. K. Kuramoto, M. Ehara, H. Nakatsuji, "Theoretical fine spectroscopy with SAC-CI general-*R* method: First-row *K*-shell ionizations and their satellites", *J. Chem. Phys.*, 122, 014304-1-7 (2005).
23. K. Kuramoto, M. Ehara, H. Nakatsuji, M. Kitajima, H. Tanaka, A. De Fanis, Y. Tamenori, K. Ueda, "C1s and O1s photoelectron spectra of formaldehyde with satellites: theory and experiment", *J. Electron Spectrosc. Relat. Phenom.* 142, 253-259 (2005).
24. M. Kato, M. Hada, R. Fukuda, H. Nakatsuji, "Relativistic Configuration interaction and Coupled Cluster Methods Using Four-component Spinors: Magnetic shielding constant of HX and CH₃X (X=F, Cl, Br, I)", *Chem. Phys. Lett.* 408, 1150-156 (2005).
25. T. Yamahsita, S. Kato, "Excited state electronic structures and dynamics of NOCl: A new potential function set, absorption spectrum, and photodissociation mechanism", *J. Chem. Phys.*, 121, 2105-2116 (2004).
26. T. Yonehara, T. Yamamoto, S. Kato, "Cumulative reaction probabilities for the unimolecular dissociation and isomerization reactions of formaldehyde", *Chem. Phys. Lett.*, 393, 98-101 (2004).
27. H. Tanimura, M. Hada, "Nuclear Magnetic Shielding Constants of Halogens in X- and XO₄- (X=F, Cl, Br, I) - Relativistic and Electron-Correlation Effects -", *J. Comp. Chem. Japan*, 3, 153-158 (2004).
28. J. Wan, H. Nakatsuji, "Theoretical study of the singlet and triplet vertical electronic transitions of styrene by the symmetry adapted cluster-configuration interaction method", *Chem. Phys.*, 302, 125-134 (2004).
29. K. Ueda, M. Hoshino, T. Tanaka, M. Kitajima, H. Tanaka, A. De Fanis, Y. Tamenori, M. Ehara, F. Oyagi, K. Kuramoto, H. Nakatsuji, "Symmetry-resolved vibrational spectra of carbon K-shell photoelectron satellites in carbon monoxide: experiment and theory", *Phys. Rev. Lett.* 94, 243004 1-4 (2005).
30. M. Ehara, M. Ishida, H. Nakatsuji, "Outer- and inner-valence ionization spectra of CO and N₂: SAC-CI general-*R* study", *Collection of Czechoslovak Chemical Communications*, 70, 881-904 (2005).

31. M. Ehara, Y. Ohtsuka, H. Nakatsuji, M. Takahashi, Y. Udagawa, "Theoretical fine spectroscopy with SAC-CI method: outer- and inner-valence ionization spectra of furan, pyrrole, and thiophene", *J. Chem. Phys.* 122, 234319-1-10 (2005).
32. P. Poolmee, S. Hannongbua, M. Ehara, H. Nakatsuji, "SAC-CI Theoretical Investigation on Electronic Structure of Fluorene-Thiophene Oligomers", *Polymer*, 46, 6474-6481 (2005).
33. M. Ehara, M. Nakata, H. Nakatsuji, "Valence ionized states with low-lying satellites: $n-\pi^*$ and $\pi-\pi^*$ transitions in 4π -electron molecules", *Mol. Phys.* in press.
34. Y. Honda, M. Hada, M. Ehara, H. Nakatsuji, "Theoretical studies on magnetic circular dichroism by the finite perturbation method and relativistic corrections", *J. Chem. Phys.* 123, 164113-1-9 (2005).
35. J. Hasegawa, H. Nakatsuji, "Generalization of the Projection Space Improves the SAC-SD (symmetry-adapted cluster-singles and doubles) Method in Bond-breaking Systems", *Chem. Letters*. 34, 1356-1357 (2005).
36. R. Fukuda and H. Nakatsuji, "Quasirelativistic theory for the magnetic shielding constant. III. Quasirelativistic second-order Møller–Plesset perturbation theory and its application to tellurium compounds", *J. Chem. Phys.* 123, 044101-1-10 (2005).
37. M. Ehara, J. Hasegawa, H. Nakatsuji, "SAC-CI Method Applied to Molecular Spectroscopy", in *Theory and Applications of Computational Chemistry: The First 40 Years, A Volume of Technical and Historical Perspectives*, edited by C.E. Dykstra, G. Frenking, K.S. Kim, G.E. Scuseria. (Elsevier, Oxford, 2005).
38. M. Matsumoto, K. Ueda, E. Kukk, H. Yoshida, T. Tanaka, M. Kitajima, H. Tanaka, Y. Tamenori, K. Kuramoto, M. Ehara, and H. Nakatsuji, "Vibrationally resolved C and O 1s photoelectron spectra of carbon monoxide", *Chem. Phys. Lett.* 417, 89-93 (2006).
39. S. Arulmozhiraja, R. Fukuda, M. Ehara, H. Nakatsuji, "Electronic Spectra and Photodissociation of Vinyl Chloride - A SAC-CI Study", *J. Chem. Phys.* in press.
40. Y. Ohtsuka and H. Nakatsuji, "Inner-Shell Ionizations and Satellites Studied by the Open-Shell

Reference (OR) Symmetry-Adapted Cluster (SAC)/SAC Configuration Interaction (CI) Method”, J. Chem. Phys. in press.

4. 生体反応系の電子論とダイナミックスの解明

1. T. Miyahara, H. Nakatsuji, and J. Hasegawa, A. Osuka, N. Aratani, and A. Tsuda, “Ground and Excited States of Linked and Fused Zinc Porphyrin Dimers: SAC-CI Study”, J. Chem. Phys., 117, 11196-11207 (2002).
2. W. Nowak, Y. Ohtsuka, J. Hasegawa, H. Nakatsuji, “Density Functional Study on Geometry and Electronic Structure of Nitrile Hydratase Active Site Model”, Intern. J. Quantum. Chem., 90, 1174-1187 (2002).
3. A.K. Das, J. Hasegawa, T. Miyahara, M. Ehara and H. Nakatsuji, “Electronic Excitations of the Green Fluorescent Protein Chromophore in its Protonation States: SAC/SAC-CI Study”, J. Comp. Chem., 24, 1421-1431 (2003).
4. J. Hasegawa, M. Ishida, and H. Nakatsuji, “Energetics of the Electron Transfer from Bacteriopheophytin to Ubiquinone in the Photosynthetic Reaction Center of Rhodospseudomonas Viridis: Theoretical Study”, J. Phys. Chem. B, 107, 838-847 (2003).
5. T. Ishida, S. Kato, “Theoretical Perspectives on the Reaction Mechanism of Serine Proteases: The Reaction Free Energy Profiles of the Acylation Process.”, J. Am. Chem. Soc., 125, 12035-12048 (2003).
6. Masahiko Hada, “Quantum-Chemical Calculations for Paramagnetic ^{13}C NMR Chemical Shifts of Iron-Bound Cyanide Ions of Iron Porphyrins in Ground and Low-Lying Excited States Containing Ferric $(d_{xy})^2(d_{xz,yz})^3$ and $(d_{xy})^1(d_{xz,yz})^4$ Configurations”, J. Am. Chem. Soc., **126**(2), 486-487, 2004.
7. J. Hasegawa, K. Takata, T. Miyahara, S. Neya, M. J. Frisch, H. Nakatsuji, “Excited States of Porphyrin Isomers and Porphycene Derivatives: A SAC-CI Study”, J. Phys. Chem. A, 109, 3187-3200 (2005).
8. J. Hasegawa, T. Kimura, H. Nakatsuji, “Aza-substitution effect on the Q-band excitations of free-base porphyrin, chlorin, and bacteriochlorin: SAC-CI theoretical study”, Journal of Porphyrins and Phthalocyanines, 9, 305 (2005).

9. T. Ishida, S. Kato, "Role of Asp102 in the Catalytic Relay System of Serine Proteases: A Theoretical Study", *J. Am. Chem. Soc.*, 126, 7111-7118 (2004).

10. H. Nakashima, J. Hasegawa, H. Nakatsuji, "Reversible binding of dioxygen to Fe-porphyrin complex", *J. Comp. Chem.* 2005, in press.

11. J. Hasegawa, H. Nakatsuji, "Mechanism and Excited States and Electron Transfer Mechanism in the Photosynthetic Reaction Center of Rhodobacter Sphaeroides: SAC-CI Theoretical Study", *Chemistry Letters*. 34, 1242-1243 (2005).

12. J. Hasegawa, M. Isshiki, K. Fujimoto, H. Nakatsuji, "SAC-CI theoretical study on the structure of phytychromobilin in the Pr and Pfr forms", *Chemical Physics Letters*, 410, 90-93 (2005).

13. K. Fujimoto, J. Hasegawa, S. Hayashi, S. Kato, H. Nakatsuji, "Mechanism of color-tuning in retinal proteins: SAC-CI and QM/MM study", *Chemical Physics Letters*, 414, 239-242 (2005).

5. 凝縮系における反応の電子論とダイナミックス

1. A. Morita and S. Kato, "The Charge Response Kernel with Modified Electrostatic Potential Charge Model", *J. Phys. Chem. A.*, 90, 3909-3916 (2002).

2. S. Iuchi, A. Morita, and S. Kato, "Molecular Dynamics Simulation with the Charge Response Kernel: Vibrational Spectra of Liquid Water and N-Methylacetamide in Aqueous Solution", *J. Phys. Chem. B*, 106, 3466-3476 (2002).

3. K. Ohmiya and S. Kato, "Solution reaction path Hamiltonian based on reference interaction site model self-consistent field method: Application to Menshutkin-type reactions", *J. Chem. Phys.*, 119, 1601-1610 (2003).

4. S. Yamazaki and S. Kato, "Excited-state proton transfer of 1-[(dimethylamino)methyl]-2-naphthol in acetonitrile solvent: RISM-SCF and MRMP approach", *Chem. Phys. Lett.*, 386, 414-418 (2004).

5. H. Sato, F. Hirata, and S. Sakaki, "Distortion of Electronic Structure in Solvated Molecules: Tautomeric Equilibrium of 2-Pyridone and 2-Hydroxypyridine in Water Studied by the RISM-SCF/MCSCF Method", *J. Phys. Chem. A*, 108, 2097-2102 (2004).

6. H. Sato and S. Sakaki, "Comparison of Electronic Structure Theories for Solvated Molecule:

RISM-SCF versus PCM”, *J. Phys. Chem. A*, **108**, 1629-1634 (2004).

7. S. Iuchi, A. Morita, and S. Kato, “Potential energy surfaces and dynamics of Ni²⁺ ion aqueous solution: Molecular dynamics simulation of the electronic absorption spectrum”, *J. Chem. Phys.*, **121**, 8446-8457 (2004).

6. 表面—分子相互作用系と触媒反応の電子論

1. H. Sakurai and S. Kato, “Theoretical Study of the Metal Oxidation Reaction $Ti + O_2 \rightarrow TiO + O$: Ab Initio Calculation of the Potential Energy Surface and Classical Trajectory Analysis”, *J. Phys. Chem. A.*, **106**, 4350-4357 (2002).

2. Y. Goto, N. Nakashima, M. Takafuji, S. Sakaki, and H. Ihara, “Selectivity Enhancement for Diastereomer Separation in RPLC Using Crystalline-Organic Phase-Bounded Silica Instead of Simply-Hydrophobized Silica Chromatographia”, *Chromatographia*, **56**, 19-23 (2002).

3. Y. Musashi and S. Sakaki, “Theoretical Study of Rhodium(III)-Catalyzed Hydrogenation of Carbon Dioxide into Formic Acid. Significant Differences in Reactivity among Rhodium(III), Rhodium(I), and Ruthenium(II) Complexes”, *J. Am. Chem. Soc.*, **124** (25), 7588-7603 (2002).

4. S. Sakaki, M. Sumimoto, M. Fukuhara, M. Sugimoto, H. Fujimoto, and S. Matsuzaki, “Why Does the Rhodium-Catalyzed Hydrosilylation of Alkenes Take Place Through a Modified Chalk-Harrod Mechanism? A Theoretical Study”, *Organometallics*, **21** (8), 3788-3802 (2002).

5. T. Tomita, T. Takahama, M. Sugimoto, and S. Sakaki, “Why is the Nickel(II) diphenyldiimine Complex the Best Catalyst for Polymerization of Ethylene in Three Kinds of Cationic Nickel(II) Complexes, $[Ni(CH_3)L]^+$ (L = Diphenyldiimine, 2,2'-Bipyridine, or 1,2-Diphosphinoethane)? A Theoretical Study”, *Organometallics*, **21** (18), 3788 – 3802 (2002).

6. M. Sumimoto, S. Sakaki, S. Matsuzaki, and H. Fujimoto, “Significant differences in electronic structure among X-, α - and β -forms of lithium phthalocyanine”, *Dalton Trans.*, 31-33 (2002).

7. T. Hamada, S. Tanaka, H. Koga, Y. Sakai, and S. Sakaki, “Kinetic study of the photo-induced electron transfer reaction between ruthenium(II) complexes of 2,2'-bipyridine derivatives and methyl viologen. Effects of bulky substituents introduced onto 2,2'-bipyridine”, *Dalton Trans.* 692-698 (2002).

8. Hydrogenation of carbon dioxide catalyzed by transition metal complexes —Theoretical Approach to Catalytic Cycle and Elementary Processes, S. Sakaki, In "Catalysis by Metal Complexes vol. 25; Computational Modelling of Homogeneous Catalysis", Ed. by Feliu Maseras and Agusti Lledos, Kluwer, 2002, pp.79-106.
9. H. Koga, T. Hamada, and S. Sakaki, "Synthesis of methylviologen-pendent iron porphyrins as functional model of reduction enzyme and its application to six electron reduction of nitrobenzene to aniline", Dalton Trans., 1153-1160 (2003).
10. H. Koga, T. Arai, T. Hamada, and S. Sakaki, "Application of metalloporphyrins and methylviologen-pendant iron porphyrin to reduction of diphenylsulfoxide", J. Mol. Cat. (A), 200, 223-228 (2003).
11. S. Sakaki, "Theoretical Study of C-H Bond Activation and Related Reaction", Bull. Korean Chem. Soc., 24, 829 (2003).
12. H. Tamura, H. Yamazaki, H. Sato, and S. Sakaki, "Iridium-Catalyzed Borylation of Benzene with Diboron. Theoretical Elucidation of Catalytic Cycle Including Unusual Iridium(V) Intermediates", J. Am. Chem. Soc., 125 (51), 16114 - 16126 (2003).
13. H. Koga, T. Hamada, and S. Sakaki, "Synthesis of methylviologen-pendent iron porphyrins as functional model of reduction enzyme and its application to six electron reduction of nitrobenzene to aniline", Dalton Trans., 1153-1160 (2003).
14. S. Sakaki, T. Takayama, M. Sumimoto, and M. Sugimoto, "Theoretical Study of Cp₂Zr-Catalyzed Hydrosilylation of Ethylene. Reaction Mechanism Including New σ -Bond Activation", J. Am. Chem. Soc., 126, 3332-3348 (2004).
15. M. Sumimoto, N. Iwane, T. Takahama, and S. Sakaki, "Theoretical Study of Trans-metallation Process in Palladium-Catalyzed Borylation of Iodobenzene with Diboron", J. Am. Chem. Soc., 126, 10457-10471 (2004).
16. S. Nakajima, D. Yokogawa, Y. Nakao, H. Sato, and S. Sakaki, "Bis(μ -silylene)-bridged dinuclear rhodium(0) complex and Its Palladium(0) and Platinum(0) Analogues. Theoretical Study of their Electronic Structure, Bonding Nature, and Interconversion between μ -Disilene-bridged Form and bis(μ -silylene)-bridged Form", Organometallics, 23, 4672-4681 (2004).

17. Y. Ohnishi, T. Matsunaga, Y. Nakao, H. Sato, and S. Sakaki, "Ruthenium(II)-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. Theoretical Study of Real Catalyst, Ligand Effects, and Solvation Effects", *J. Am. Chem. Soc.*, 127, 4021-4032 (2005).

18. H. Nakatsuji, N. Matsumune, and K. Kuramoto, "Theoretical surface spectroscopy of NO on Pt(111) surface with DAM and SAC-CI method", *J. Chem. Theo. Comp.*, 1, 239-247 (2005).

19. Chiral Photochemistry ed. by Y. Inoue Chapter 7. Chiral Photochemistry with Transition-metal Complexes

Shigeyoshi Sakaki and Taisuke Hamada, Marcel Dekker, Inc. 2004

20. Theoretical Studies of C-H σ -Bond Activation and Related Reactions by Transition-metal Complexes, Shigeyoshi Sakaki, in *Topics Organomet. Chemistry*, 12, 31-78 (2005), in press.

7. その他

1. Z. Hu, R. J. Boyd, and H. Nakatsuji, "Molecular Structure and Excited States of $CpM(CO)_2$ ($Cp=5-C_5H_5$; $M=Rh, Ir$) and $[Cl_2Rh(CO)_2]^-$. Theoretical Evidence for a Competitive Charge Transfer Mechanism", *J. Am. Chem. Soc.*, 124, 2664-2671 (2002).

2. E. S. Kryachko and H. Nakatsuji, "Ab Initio Study of Lower Energy Phenol-Water 1^1N ", *J. Phys. Chem. A*, 106, 731-742 (2002).

3. H. Yamashita, S. Takada, M. Hada, H. Nakatsuji, and M. Anpo, "Experimental Study and Ab Initio Molecular Orbital Calculation on the Photolysis of n-butyrophenone Included within the Alkali Metal Cation-exchanged ZSM-5 Zeolite", *J. Photochem. Photobiol. A*, 160, 37-42 (2003).