

いわた すえひろ
岩田 末廣

研究テーマ: 「分子間相互作用理論とその分子クラスターへの応用」

<学歴> 1964/3 理学修士 東京大学化学系研究科化学専攻(長倉三郎教授指導)
1967/3 理学博士 東京大学理学系研究科化学専攻(長倉三郎教授指導)

<職歴>	1967/4-1981/3	研究員	理化学研究所
	1972/2-1973/8	博士研究員	ロチェスター大学 (諸熊教授)
	1973/9-1975/3	博士研究員	シカゴ大学 (フリード教授)
	1979/4-1981/3	客員助教授	分子科学研究所
	1981/4-1986/3	助教授	慶應義塾大学理工学部 化学科
	1986/4-1993/12	教授	慶應義塾大学理工学部 化学科
	1994/1-2000/3	教授	分子科学研究所
	1994/1-1994/9	客員教授	慶應義塾大学理工学部 化学科
	1994/4-2000/3	センター長	分子科学研究所 計算機センター
	1997/5-1999/3	客員教授	東京大学理学研究科化学専攻
	2000/4-present	名誉教授	分子科学研究所
	2000/4-present	名誉教授	総合研究大学院大学
	2000/4-2001/3	教授	広島大学大学院理学研究科化学専攻
	2000/11-2001/3	教授(併任)	大学評価学位授与機構
	2001/4-2004/4	教授	大学評価学位授与機構
	2001/4-2001/9	教授(併任)	広島大学大学院理学研究科化学専攻
	2002/4-2003/3	客員教授	東北大学多元物質科学研究所
	2004/5-2008/3	特任教授	広島大学大学院理学研究科
	2004/5-2005/3	客員教授	大学評価学位授与機構
	2008/4-present	フェロー	(財)豊田理化学研究所
	2008/4-2009/3	特任教授(非常勤)	広島大学大学院理学研究科

学会および社会的活動

財団法人豊田理化学研究所 フェロー 岩田未廣

2009年8月現在

専門分野

理論化学・量子化学・計算化学

所属学会

日本化学会、分子科学学会、日本物理学会、Amer.Phys.Soc

受賞

日本化学会賞 2000年3月

国際学会の組織委員

第三回世界理論有機化学会議(3rd WATOC)プログラム委員会委員長:1993.7(豊橋)

Symposium "Computational Quantum Chemistry" in PacfiChem'95 : 1995.12 (Hawaii)

Symposium "In the Frontier of Quantum Chemistry and Chemical Reactions" 1999, May, (Atlanta)

Japan-US Information Exchange Seminar "Photoconversion and Photosynthesis: Past, Present and Perspective" 1999, Nov. (Okazaki)

IMS COE international conference "Interplay of Theories and Experiments in Structural Analysis of Molecular Clusters" 1999 Dec. (Okazaki)

Symposium "Solvated Molecules and Ions: from Clusters to Condensed Phases" in PacfiChem2000 : 2000.Dec. (Hawaii)

文部省、学審等の委員

日本化学会関東支部委員 (1976-1978)

日本化学会学会賞等選考委員 (1991-1992)

岡崎国立共同研究機構・分子科学研究所 運営協議会(外部委員) 人事部会委員 (1989-1993)

岡崎国立共同研究機構・分子科学研究所 理論研究系外部評価委員(1993)

学術振興会特別研究員等審査会専門委員 (1994-1995)

通産省産業技術部会・原子分子極限操作技術分科会委員 (1992-1998)

慶應義塾大学大型研究助成審査委員 (1994-2006)

東京工業大学総合情報処理センター外部評価委員 (1995-1995)

文部省科学研究費専門委員(第1段 物理化学) (1996-1997)

日本化学会学術賞等選考委員 (1996-1997)

東京大学物性研究所運営協議会委員 (1996-1997)

北海道大学理学研究科化学専攻 外部評価委員 (1998)

学術振興会特別研究員等審査会専門委員 (2000-2001)

山田科学財団審査員(2001 - 現在)

仁科記念財団選考委員(2002—2007)

林女性自然学者研究助成基金選考委員(2002—2004)

21世紀COEプログラム 分野別審査・評価部会 化学・材料専門委員(2002, 2004, 2007)

大学院教育改革支援プログラム委員会分野別審査部会専門委員(書面審査委員)(2006, 2007)

東北大学工学研究科・工学部外部評価委員(2006)

日本化学会学会賞等選考委員 (2006-2007)

主要研究成果

		関連文献番号
I	多電子理論の開発	
1	分子間相互作用理論の開発	220, 219, 217, 215, 212, 203
2	1次元鎖結晶軌道法のエネルギー勾配法	180, 179, 176
3	電子相關計算に適した積分近似法	137, 129, 119
4	配置間相互作用法による分極率の直接計算法	88, 65, 59
5	新しい解析法による酸化数概念の検討	67, 62, 56, 47
6	原子価型空軌道による多参照配置間相互作用法	52, 60
7	Fock 空間多参照摂動理論と半経験電子理論の基礎付け	36, 31, 30, 25, 24
8	電子-空孔対法の開発	26, 13
II	分子の構造・分光・反応の量子化学	
1	大気環境分子の反応と分光	207, 204, 198
2	OH ラジカルと大気中有機化合物の反応	204, 201, 196, 178, 164, 110, 94, 79
3	二、三原子分子励起状態の精密計算	125, 107, 93, 86
4	実験で得にくい遷移確率の絶対値の精密計算	112, 95, 82
5	星間空間におけるイオン分子反応	
6	電荷移動錯体形成による赤外吸収強度変化	
III	分子クラスターの構造、反応、振動分光	総合報告 23, 24
1	電子-水素結合概念の提唱	214, 199, 197
2	クラスター固有の新しい化学結合	193, 175
3	クラスターの構造、振動分光	195, 144, 136, 130, 101
4	クラスター内反応	193, 192, 170, 163, 118, 117
5	クラスターのイオン化	187, 83, 81
6	2成分元素クラスターの構造	168, 166, 159, 121, 120, 116, 99
7	クラスター内電子遷移と光解離	185, 174, 103, 85
8	非断熱遷移を伴うクラスター内過程	185, 142, 113
9	ab initio MO - Monte-Carlo シミュレーション	190, 177, 163
IV	高い励起状態の量子化学	
1	系統的な光電子スペクトルの解析	105, 102, 58, 49, 40
	光電子スペクトル handbook	総合報告 19, 5
2	内殻電子の励起・イオン化と化学結合	73, 64, 54, 41, 37
3	極短波長エキシマーレーザーの探索	96, 87, 76, 66
	63nm にエキシマー発光する HeK ⁺ 系の提案	
V	初期の研究課題(留学以前)	
1	電荷移動(CT)型三重項の実験的発見	21, 11, 8, 7, 6, 5, 4
	CT 錯体の発光スペクトル研究の先鞭	
2	多原子分子光電子スペクトルの角度分布の理論計算	27
3	パイ電子理論による電子スペクトルの解析	38, 32, 23, 19, 12, 10
	有機ラジカルスペクトル解析	

岩田論文リスト

原著論文

- 221 Deuteration effects on the enthalpy and entropy changes in encapsulation of the methyl-containing guest molecules in molecular cages: Importance of increase of the internal rotation barrier, Suehiro Iwata, Takaharu Haino, 豊田理研研究報告, (2009) 63-77
- 220 Absolutely Local Excited Orbitals in the Higher Order Perturbation Expansion for Molecular Interaction, Suehiro Iwata, J. Phys. Chem. B. 112 (2008) 16104-16109
- 219 Perturbation expansion theory corrected from basis set superposition error II. Charge-transfer, pair correlation and dispersion terms. Suehiro Iwata and Takeshi Nagata, Theor. Chem. Acc. 117 (2007) 137-147
- 218 Theoretical studies of group 1 metal complexes with hydrogen fluoride, M(HF)_n, M=Li, Na, and K: A new type of electrides, Suehiro Iwata, J. Phys. Chem. A, 111 (2007) 7499-7503
- 217 The Single Excitation Perturbation Expansion Theory Based on the Locally Projected Molecular Orbitals for Molecular Interaction: Comparison with the Counterpoise Corrected Energy. Suehiro Iwata, Chem. Phys. Letters, 431 (2006) 204-209
- 216 Franck-Condon factors based on anharmonic vibrational wave functions of polyatomic molecules. Valerie Rodriguez-Garcia,¹ Kiyoshi Yagi, Kimihiko Hirao, Suehiro Iwata, and So Hirata, J. Chem. Phys. 125 (2006) 014109-1 - 014109-9
- 215 Locally projected molecular orbital theory for molecular interaction with a high-spin open shell molecule, Suehiro Iwata, J. Theor. Comp. Chem. 5 (2006) 819-833
- 214 Theoretical study of photoabsorption cross section of water cluster anions: The size and isomer dependences, Suehiro Iwata and Feiwu Chen, J. Electron Spectrosc. Relat. Phenom. 142 (2005) 277-281
- 213 Noble gas clusters doped with a metal ion I. Ab initio studies of Na⁺Ar_n, Takeshi Nagata, Mutsumi Aoyagi, and Suehiro Iwata, J. Phys. Chem. 108 (2004) 683-690
- 212 Perturbation expansion theory corrected from basis set superposition error I. Locally projected excited orbitals and single excitations. Takeshi Nagata and Suehiro Iwata, J. Chem. Phys. 120 (2004) 3555-3563
- 211 Theoretical studies on the molecular dependence of bond dissociation after core excitations II: CH₃CO(CH₂)_nCN, n=0-3, Osamu Takahashi, Masanori Joyabu, Masaki Mitani, Ko Saito and Suehiro Iwata, J. Comp. Chem. 24 (2003) 1329-1335
- 210 A theoretical study of Si₄H₂ cluster with ab initio and density functional methods, Wen-Ning Wang, Hai-Rong Tang, Kang-Nian Fan, Suehiro Iwata, J. Chem. Phys. 114 (2001) 1278-1285
- 209 Theoretical molecular Auger spectra with electron population analysis. Masaki Mitani, Osamu Takahashi, Ko Saito and Suehiro Iwata, J. Electron Spectrosc. Relat. Phenom. 128 (2003) 103-117
- 208 Electronic spectra and structures of solvated NH₄ radicals, NH₄(NH₃)_n (n=1 – 8). Shinji Nonose, Tomokazu Taguchi, Fenwu Chen, Suehiro Iwata, Kiyokazu Fuke, J. Phys. Chem. A106 (2002) 5242-5248
- 207 Theoretical study on the weakly-bound complexes in the reactions of hydroxyl radical with saturated hydrocarbons (methane, ethane and propane). Tomohiro Hashimoto, Suehiro Iwata, J. Phys. Chem. A106 (2002) 2652-2658
- 206 A new time-independent perturbation theory for the multireference problem. Fenwu Chen, E.R. Davidson Suehiro Iwata, Int. J. Quantum Chem. 86 (2002) 256-264
- 205 Theoretical studies on the molecular dependence of the bond dissociation after the core excitations: CH₃OCO(CH₂)_nCN, n=0,1,2. Osamu TAKAHASHI, Masaki MITANI, Masanori JOYABU, Ko SAITO and Suehiro IWATA, J. Electron Spectrosc. Relat. Phenom. 120 (2001) 137-148
- 204 Accurate evaluation of Einstein's A and B coefficients of rovibrational transitions for carbon monoxide: Spectral simulation of Δv=2 rovibrational transitions in the solar atmosphere observed by a satellite, Kazutoshi Okada and Suehiro Iwata, J. Quantitative Spectroscopy and Radiative Transfer, 72 (2002) 813-825
- 203 Basis set superposition error free self-consistent field method for molecular interaction in multi-component systems: Projection operator formalism, T. Nagata, O. Takahashi, K. Saito and S. Iwata,

- 202 Mechanism of ion desorption reaction of PMMA thin film induced by core excitation, E. O. Sako, Y. Kanameda, E. Ikenaga, M. Mitani, O. Takahashi, K. Saito, S. Iwata, S. Wada, T. Sekitani and K. Tanaka, J. Electron Spectrosc. Relat. Phenom. 114-116 (2001) 591-596.
- 201 Spectral density calculation by using the Chebyshev expansion, Tsutomu Ikegami and Suehiro Iwata, J. Comp. Chem. 23 (2002) 310-318
- 200 Theoretical study of multidimensional proton tunneling in the excited state of tropolone, Marek J. Wojcik, Hiroki Nakamura, Suehiro Iwata, Wiktor Tatara, J. Chem. Phys. 112 (2000) 6322-6328
- 199 The electron-hydrogen bonds and the OH harmonic frequency shifts in water cluster complexes with a group 1 metal atom, $M(H_2O)_n$ ($M=Li$ and Na), Takeshi Tsurusawa and Suehiro Iwata, J. Chem. Phys., 112 (2000). 5705-5710
- 198 Ab initio MO study of A, D and third $^2\Pi$ states of CO^+ , Kazutoshi Okada and Suehiro Iwata, J. Elect. Spectr Related Phenom. 108 (2000) 225-234
- 197 Theoretical studies of the water cluster anions containing the $OH\{e\}HO$ structure: energies and harmonic frequencies, Takeshi Tsurusawa and Suehiro Iwata, Chem. Phys. Letters, 315 (2000) 433-440
- 196 Accurate potential energy and transition dipole moment curves of several electronic states of CO^+ , Kazutoshi Okada and Suehiro Iwata, J.Chem.Phys. 112 (2000) 1804-1808
- 195 Theoretical study of vibrational spectra for $Cl(H_2O)$: Temperature dependence and the influenced of Ar_n ($n=1-3$), Katsuhiko Satoh and Suehiro Iwata, Chem.Phys.Letters, 312 (1999) 522-529
- 194 Electronic Isomers in $[(CO_2)_nROH]^-$ cluster anions. II. Ab initio calculations, Morihisa Saeki, Tatsuya Tsukuda, Suehiro Iwata and Takashi Nagata, J.Chem.Phys. 111 (1999) 6333-6343
- 193 Theoretical studies of structures and ionization threshold energies of water cluster complexes with a group 1 metal, $M(H_2O)_n$ ($M=Li$ and Na), Takeshi Tsurusawa and Suehiro Iwata, J.Phys.Chem. A 103 (1999) 6134-6141
- 192 Theoretical studies of $[Si_4NO]^-$ with ab initio MO and DFT methods, Wen-Ning Wang, Hai-Rong Tang, Kang-Nian Fan and Suehiro Iwata, Chem.Phys.Letters, 310 (1999) 313-322
- 191 On connection between the reference interaction site model integral equation theory and the partial wave expansion of molecular Orstein-Zernike equation, Seiichiro Tenno and Suehiro Iwata, J.Chem.Phys. 111 (1999) 4865-4868
- 190 Structures and photoelectron spectroscopies of $Si_2C_2^-$ studied with ab initio multicanonical Monte Carlo simulation, Pradipta Bandyopadhyay, Seiichiro Ten-no and Suehiro Iwata, J.Phys.Chem.A 103 (1999) 6442-6447
- 189 Size-extensive calculations of static structure factors from the coupled cluster singles and doubles model, Noboru Watanabe, Seiichiro Ten-no, Sourav Pal, Suehiro Iwata and Yasuo Udagawa, J.Chem.Phys. 111 (1999) 827-832
- 188 The heat of formation of the SiF_2^{++} dication: A theoretical prediction, Jan Hrusak, Zdenek Herman and Suehiro Iwata, Int.J.Mass Spectr. 192 (1999) 165-171
- 187 Theoretical study on spectroscopic properties of positive, neutral and negative species of BCl_2 and $AlCl_2$: The stability of the neative species, Kyoung K.Baeck, Heechol Choi and Suehiro Iwata, J.Phys.Chem. A 103 (1999) 6772-6777
- 186 Investigation of the potential energy surfaces for the ground X^1A_1 and excited C^1B_2 electronic states of SO_2 , Petr Nachtigall, Jan Hrusak, Ota Bludsky and Suehiro Iwata, Chem.Phys.Letters, 303 (1999) 441-1446
- 185 Photodissociation dynamics of argon cluster ions, Tsutomu Ikegami and Suehiro Iwata,, J.Chem.Phys. 110 (1999) 8492-8500
- 184 Ab initio MO studies of van der Waals molecule $(N_2)_2$: Potential energy surface and internal motion, Akira Wada, Hideto Kanamori and Suehiro Iwata, J.Phys.Chem. 109 (1998) 9434-9438
- 183 Theoretical studies of internal methyl rotations in m-xylene: Comparison of Franck-Condon factors

- with the experimental spectra, Tadayoshi Suzuki, Tsutomu Ikegami, Masaaki Fujii and Suehiro Iwata, J.Molec.Struc.(THEOCHEM), 461-462 (1999) 79-90
- 182 Generalization of the coupled-cluster response theory to multireference expansion spaces: an application of the coupled-cluster singles and doubles effective Hamiltonian, Seiichiro Ten-no, Suehiro Iwata, Sourav Pal and Debasish Mukherjee, Theor. Chem. Accounts, 102 (1999) 252
- 181 Model study of H-bonded ROH... $(\text{NH}_3)_5$ clusters: a search for possible ground state proton transfer species, Michail V. Vener and Suehiro Iwata, Chem.Phys.Letters, 292 (1998) 87-91
- 180 Ab initio Hartree-Fock and Density Functional Studies on the Structures and Vibrations of an Inite Hydrogen Fluoride Polymer, So Hirata and Suehiro Iwata, J.Phys.Chem. 102 (1998) 8426-8436
- 179 Analytical energy gradients in second-order Moller-Plesset perturbation theory for extended systems, So Hirata, Suehiro Iwata, J.Chem.Phys. 109 (1998) 4147-4155
- 178 A theoretical study of the electronic structure and spectroscopic properties of the low-lying electronic states of the molecule AlSi, Fernando R. Ornellas and Suehiro Iwata, Chem.Phys. 232 (1998) 95-110
- 177 Ab initio Monte Carlo simulation using multicanonical algorithm: temperature dependence of the average structure of water dimer, Pradipta Bandyopadhyay, Seiichiro Ten-no and Suehiro Iwata, Mol. Phys. 96 (1999) 349-358
- 176 Analytical second derivatives in ab initio Hartree-Fock crystal orbital theory of polymers, So Hirata, Suehiro Iwata, J.Molec.Structure (THEOCHEM), 451 (1998) 121 - 134
- 175 Dipole-bound and interior electrons in water dimer and trimer anions: ab initio MO studies, Takeshi Tsurusawa and Suehiro Iwata, Chem.Phys. Letters 287 (1998) 553-562
- 174 Theoretical assignment of the photo-dissociation excitation spectra of the Mg^+ ion complexes with water clusters: Multi-reference CI studies, Hidekazu Watanabe and Suehiro Iwata, J.Chem.Phys. 108 (1998) 10078-10083
- 173 Variety of [Fe, N, O] isomers. A theoretical study, Andreas Fiedler and Suehiro Iwata, J.Phys.Chem. 102 (1998) 3618-3624
- 172 Ab initio MO and density functional studies on the vibrational spectra of 1,4-benzoquinone, and its anion and dianion. Chang-Guo Zhan and Suehiro Iwata, Chem.Phys. 230 (1998) 45-56
- 171 Density functional crystal orbital study on the normal vibrations and phonon dispersion curves of all-trans polyethylene, Soh Hirata and Suehiro Iwata, J.Chem.Phys. 108 (1998) 7901-7908
- 170 Intracluster Reaction Dynamics of Ar_4^+ , Tsutomu Ikegami and Suehiro Iwata, "The Transition State, Theoretical Approach", Ed. by Fueno, Kodansha, Tokyo (1999) 115-128
- 169 Static structure factor and electron correlation effects studied by inelastic x-ray scattering spectroscopy, Noboru Watanabe, Hisashi Hayashi, Yasuo Udagawa, Seiichiro Ten-no and Suehiro Iwata, J. Chem. Phys. 108 (1998) 4545-4553
- 168 Geometric and electronic structures of silicon-sodium binary clusters. II., Photoelectron spectroscopy of Si_nNa_m^- cluster anions, Reiko Kishi, Hiroshi Kawamata, Yuichi Negishi, Suehiro Iwata, Atsushi Nakajima and Koji Kaya, J. Chem. Phys. 107 (1997) 10029-10043
- 167 Photoabsorption and photofragmentation studies of acyloxy iodide anion $\text{CH}_3\text{CO}_2\text{I}^-$, Morihisa Saeki, Lei Zhu, Tatsuya Tsukuda, Suehiro Iwata and Takashi Nagata, Chem.Phys.Letters, 280 (1997) 343-352
- 166 Ab initio studies on the structures, vertical electron detachment energies and stabilities of C_nP^- , Chang-Guo Zhan and Suehiro Iwata, J. Chem. Phys. 107 (1997) 7323-7330
- 165 Local hard - soft acid base principle: a critical study, Sailaja Krishnamurty, Ram Kinkar Roy, Rajappan Vertrivel, Suehiro Iwata and Sourav Pal, J.Phys.Chem. 101 (1997) 7253 - 7257
- 164 A theoretical study of the electronic structure and spectroscopic properties of the low-lying electronic states of the molecule SiB, Fernando R Ornellas and Suehiro Iwata, J.Chem.Phys. 107 (1997) 6782-6794
- 163 Theoretical prediction of intracluster reactions of $\text{B}^+(\text{H}_2\text{O})_2$ and $\text{B}^+(\text{H}_2\text{O})_3$: Hybrid procedure of ab initio MO calculations and Monte Carlo samplings., Hidekazu Watanabe, Toshio Asada and Suehiro Iwata, Bull. Chem. Soc. Jpn, 70 (1997) 2619-2629
- 162 Reaction of negatively-charged clusters of carbon dioxide with CH_3I : Formation of novel molecular anion $\text{CH}_3\text{CO}_2\text{I}$, Tatsuya Tsukuda, Morihisa Saeki, Suehiro Iwata and Takeshi Nagata,

- J.Phys.Chem. A 101 (1997) 5103-5110
- 161 Ab initio study of the isomers: HNNSi, HSiNN, and HNSiN, Fernando R. Ornellas and Suehiro Iwata, Bull.Chem.Soc.Jpn, 70 (1997) 2057-2062
- 160 Ab initio MO studies of Si_4NO^+ cluster, Wen-Ning Wang, Kang-Nian Fan and Suehiro Iwata, Chem.Phys.Letters, 273 (1997) 337-344
- 159 Geometric and electronic structures of silicon-sodium binary clusters. I. Ionization energy of Si_nNa_m , Reiko Kishi, Suehiro Iwata, Atsushi Nakajima and Koji Kaya, J.Chem.Phys. 107 (1997) 3056-3070
- 158 Ab initio MO studies of neutral and anionic SiC_n clusters (n=2 - 5), Motoki Gomei, Reiko Kishi, Atsushi Nakajima, Suehiro Iwata and Koji Kaya, J. Chem. Phys. 107 (1997) 10051-10061
- 157 Potential energy surfaces of the ground and low-lying states of HCCS and NCS: CASSCF, MRCI and CCSD(T) studies, Yumin Li and Suehiro Iwata, Chem.Phys.Letters, 273 (1997) 91-97
- 156 Theoretical study of cyclic radicals NO_x (x=2 - 6), Yumin Li and Suehiro Iwata, Chem. Phys. 219 (1997) 209-219
- 155 Density functional crystal orbital study on the normal vibrations of polyacetylenes and polymethyneimine, So Hirata and Suehiro Iwata, J.Chem.Phys. 107 (1997) 10075-10084
- 154 Portrait of diatomic FeN. A theoretical study. Andreas Fiedler and Suehiro Iwata, Chem. Phys. Letters, 271 (1997) 143-151
- 153 Ab initio study of photochemical reactions of ammonia dimer systems. Jong Keun Park and Suehiro Iwata, J. Phys. Chem. A101 (1997) 3613-3618
- 152 The ground state (${}^1\text{A}_1$) and the lowest triplet state (${}^3\text{B}_2$) of the phenyl C_6H_5^+ revisited., Jan Hrusak, Detlef Schroder and Suehiro Iwata, J. Chem. Phys. 106 (1997) 7541-7549
- 151 Comparative ab initio and hybrid DFT studies relevant to an experimental investigation of neutral and cationic [Si, P, H₂] isomers, Jan Hrusak, Detlef Schroder, Helmut Schwarz and Suehiro Iwata, Bull. Chem. Soc. Jpn. 70 (1997) 777-787
- 150 Quadratic Configuration Interaction versus Coupled Cluster Theory: Importance of Orbital Relaxation Phenomena in CuH and CuF, Jan Hrusak, Seiichiro Ten-no and Suehiro Iwata, J. Chem. Phys. 106 (1997) 7185-7192
- 149 The vibrational spectrum of H_2O_2^+ radical cation: An illustration of symmetry breaking, Jan Hrusak and Suehiro Iwata, J. Chem. Phys. 106 (1997) 4877-4888
- 148 Diazasilene (SiNN): Is there a conflict between experiment and theory? Fernando R. Ornellas, Leonardo T. Ueno and Suehiro Iwata, J. Chem. Phys 106 (1997) 151-157
- 147 Theoretical studies of cyclic isomers of HNO_x (x= 2 - 6), Yumin Li and Suehiro Iwata, Bull. Chem. Soc. Jpn, 70 (1997) 79-88
- 146 Resonance Raman and FTIR spectra of isotope-labeled reduced 1,4-benzoquinone and its protonated forms in solution, Xiaojie Zhao, Hiroshi Imahori, Chang-Guo Zhan, Yoshiteru Sakata, Suehiro Iwata and Teizo Kitagawa, J. Phys. Chem. A101 (1997) 266-631
- 145 Ab initio studies on the structures, vertical electron detachment energies and fragmentation energies of C_nB^- clusters, Chang-Guo Zhan and Suehiro Iwata, J. Phys. Chem. A101 (1997) 591-596
- 144 Molecular orbital studies of the structures and reactions of a singly charged calcium ion with water clusters, $\text{Ca}^+(\text{H}_2\text{O})_n$, Hidekazu Watanabe and Suehiro Iwata, J. Phys.Chem. A101 (1997) 487-496
- 143 Theoretical prediction of the ${}^{31}\text{P}$ NMR chemical shift pf the hexa-coordinate phosphorus intermediate for the phosphoryl ester exchange and N → O migration reactions of dimethyloxyphosphoryl-threonin, Chang-Guo Zhan and Suehiro Iwata, Chem. Letters (1997) 3-4
- 142 Size dependence of the photoabsorption spectra of Ar_n^+ , n = 4 - 25: a solvation effect on the Ar_3^+ chromophore, Tsutomu Ikegami and Suehiro Iwata, J.Chem.Phys. 105 (1996) 10734 - 10740
- 141 Structures and energetics of new nitrogen and silicon molecules: an ab initio studies of Si₂N₂, Fernando R. Ornellas and Suehiro Iwata, J. Phys. Chem. 100 (1996) 16155-16161
- 140 Hybrid procedure of ab initio molecular orbital calculation and Monte Carlo simulation for studying the intracluster reactions: Applications to $\text{Mg}^+(\text{H}_2\text{O})_n$ (n=1 - 4), Toshio Asada and Suehiro Iwata, Chem.Phys. Letters, 260 (1996) 1-6

- 139 Photoelectron spectroscopy of silicon-fluorine binary cluster anions (Si_nF_m^-), Hiroshi Kawamata, Yuichi Negishi, Reiko Kishi, Suehiro Iwata, Atsushi Nakajima and Koji Kaya, J.Chem.Phys. 105 5369-5378 (1996)
- 138 Ab initio studies of silicon and nitrogen clusters: Cyclic or linear Si_2N^- ? Fernando R. Ornellas and Suehiro Iwata, J.Phys.Chem. 100 (1996) 10919-10927
- 137 On approximating electron repulsion integrals with linear combination of atomic-electron distribution, Seiichiro Ten-no and Suehiro Iwata, Int. J. Quant. Chem. 60, S30 (1996) 1319 - 1324
- 136 Does the proton transfer reaction take place in the ground state of phenol-(H_2O)₄ cluster, Hidekazu Watanabe and Suehiro Iwata, Int. J. Quant. Chem. 60, S30 (1996) 1607-1613
- 135 Electronic and geometrical structures of silicon-M binary clusters (M= C and Na,, Reiko Kishi, Atsushi Nakajima, Suehiro Iwata and Koji Kaya, "Structures and Dynamics of Clusters", Ed. by T.Kondow, K.Kaya, A.Terasaki, Universal Academy Press, Tokyo, (1996) 607-612
- 134 Theoretical studies of molecular spectroscopies of some small clusters, Suehiro Iwata and Hidekazu Watanabe, "Structures and Dynamics of Clusters", Ed. by T.Kondow, K.Kaya, A.Terasaki, Universal Academy Press, Tokyo, (1996) 209-218
- 133 Electron-correlation effects on geometrical and electronic structures of Si_nNa clusters, Reiko Kishi, Atsushi Nakajima, Suehiro Iwata and Koji Kaya, Surface Review and Letters, 3 (1996) 365-369
- 132 Photoelectron spectroscopy of binary metal cluster anions containing sulfur atom, Atsushi Nakajima, Tetsuya Taguwa, N. Nakao, K. Hoshino, Suehiro Iwata and Koji Kaya, Surface Review and Letters, 3 (1996) 417-421
- 131 Photoelectron spectroscopy of silicon-carbon cluster anions, Atsushi Nakajima, Tetsuya Taguwa, N. Nakao, Motoki Gomei, Reiko Kishi, Suehiro Iwata and Koji Kaya Surface Review and Letters, 3 (1996) 411-415
- 130 Theoretical studies of geometric structures of phenol-water clusters and their infra-red absorption spectra in the O-H stretching region, Hidekazu Watanabe and Suehiro Iwata, J.Chem.Phys. 105 (1996) 420-431
- 129 Multi-configuration self-consistent field procedure employing linear combination of atomic-electron distributions, Seiichiro Ten-no and Suehiro Iwata, J. Chem. Phys. 105 (1996) 3604-3609
- 128 Ab initio studies on the structures, vertical electron detachment energies and fragmentation energies of C_nN^- clusters, Chang-Guo Zhan and Suehiro Iwata, J.Chem.Phys. 104 (1996) 9058-9064
- 127 Theoretical studies of carbon doped small silicon clusters: Electron affinities of Si_nC (n=2 - 5), Reiko Kishi, Motoki Gomei, Atsushi Nakajima, Suehiro Iwata and Koji Kaya, J.Chem.Phys., 104 (1996) 8593-8604
- 126 Theoretical studies of boron - water cluster ions $\text{B}^+(\text{H}_2\text{O})_n$ and aluminium - water clusters $\text{Al}^+(\text{H}_2\text{O})_n$: Isomers and intra-cluster reactions. Hidekazu Watanabe and Suehiro Iwata, J.Phys.Chem. 100 (1996) 3377-3388
- 125 Theoretical studies of the chemical processes of producing methylamine and methanol in the interstellar space, Yoko Sonoda and Suehiro Iwata, Bull.Chem.Soc.Japan, 69 (1996) 575-579
- 124 Theoretical studies of the ground and low-lying excited electronic states of the early transition metal dihydrides with state averaged MC SCF method, T. Shyunmei Fujii and Suehiro Iwata, Chem. Phys. Letters, 251 (1996) 150-156
- 123 Ab initio studies on structures of the hexa-coordinate phosphorus intermediate for the phosphoryl ester exchange and migration reactions of dimethyloxyphosphoryl-threonine, Chang-Guo Zhan and Suehiro Iwata, Chem.Phys.Letters, 247 (1995) 401-407
- 122 Theoretical studies of the internal rotation of the methyl group in o-, m-, and p-fluorotoluenes and their cations, Yoko Sonoda and Suehiro Iwata, Chem.Phys.Letters, 243 (1995) 176-182
- 121 Photoelectron spectroscopy of silicon-carbon cluster anions (Si_nC_m^-), Atsushi Nakajima, Tetsuya Taguwa, Kojiro Nakao, Motoki Gomei, Rriko Kishi, Suehiro Iwata and Koji Kaya, J. Chem. Phys. 103 (1995) 2050 – 2057
- 120 Electronic properties of silicon - M binary clusters (M = C and Na), Atsushi Nakajima, K. Nakao, Motoki Gomei, Reiko Kishi, Suehiro Iwata and Koji Kaya, Mat. Res. Soc. Sym. Proc. 358 (1995) 61 -66
- 119 Three-center expansion of electron repulsion integrals with linear combination of atomic electron distribution, Seiichiro Ten-no and Suehiro Iwata, Chem.Phys.Letters, 240 (1995) 578 - 584

- 118 Molecular orbital studies of the structures and reactions of singly charged magnesium ion with water clusters, $Mg^+(H_2O)_n$. Hidekazu Watanabe, Suehiro Iwata, Kenro Hashimoto, Fuminori Misaizu and Kiyokazu Fuke, J.Am.Chem.Soc. 117 (1995) 755-763
- 117 Reactions of Singly Charged Alkaline-Earth Metal Ions with Water Clusters: Charateristic Size Distribution of Product Ions. Masaomi Sanekata, Fuminori Misaizu, Kiyokazu Fuke, Suehiro Iwata, Kenrou Hashimoto, J.Am.Chem.Soc. 117 (1995) 747-754
- 116 Photoelectron spectroscopy of $Al_nS_1^-$ clusters (n=1 - 9), Atsushi Nakajima, Tetsuya Taguwa, Kojiro Nakao, Kuniyoshi Hoshino, Suehiro Iwata and Koji Kaya, J.Chem.Phys. 102 (1995) 660-665
- 115 Ab Initio Studies on the Structures and Vertical electron Detachment Energies of Copper-Water negative ion Clusters $Cu^-(H_2O)_n$ and $CuOH^-(H_2O)_{n-1}$. Chang-Guo Zhan and Suehiro Iwata, Chem.Phys.Letts. 232 (1995) 72-78
- 114 Photoionization electronic spectroscopy of $AlNa$, Atsushi Nakajima, Kuniyoshi Hoshino, Katsura Watanabe, Yuji Konishi, Tsutomu Konishi, Suehiro Iwata and Koji Kaya, Chem.Phys.Letters, 222 (1994) 353-357
- 113 Theoretical studies on the non-adiabatic photodissociation process of argon cluster ions Ar_7^+ , Tsutomu Ikegami and Suehiro Iwata, Int.J.Quantum.Chem. Symp. 28 (1994) 529-539
- 112 Theoretical studies of ammonia-halogen and methylamine-halogen complexes: Geometries, harmonic vibrational frequencies and their infrared intensities, and excited states of ammonia-chlorine monofluoride complex, Takao Kobayashi, Hidenori Matsuzawa, Suehiro Iwata, Bull.Chem.Soc.Jpn, 67 (1994) 3172-3178
- 111 Photoelectron spectroscopy of AlS^- diatomic anion, Atsushi Nakajima, Tetsuya Taguwa, Kojiro Nakao, Kuniyoshi Hoshino, Suehiro Iwata and Koji Kaya, Chem.Lett., (1994) 1525-1528
- 110 Potential Energy Surfaces of Some Low-Lying States of Fluoroformyl Radical FCO. Shinkoh Nanbu, Masahiro Gomyo and Suehiro Iwata, Chem.Phys. 184 (1994) 97-106
- 109 Photodissociation study on $Mg^+(H_2O)_n$, n=1 - 5: Electronic structure and photoinduced intracluster reaction, Fuminori Misaizu, Masaomi Sanekata, Kiyokazu Fuke and Suehiro Iwata, J.Chem.Phys., 100 (1994) 1161-1170
- 108 Theoretical Study of Silicon-Sodium Binary Clusters: Geometrical and Electronic Structures of Si_nNa (n=1,7), Reiko Kishi, Atsushi Nakajima, Suehiro Iwata and Koji Kaya, Chem.Phys.Letters, 224 (1994) 200-206
- 107 Molecular orbital study of the ion-molecule reactions producing the hydrocarbons in interstellar space, Yoko Sonoda, Suehiro Iwata and Yoshihiro Osamura, Bull.Chem. Soc. Jpn., 66 (1993) 3345-3351
- 106 Theoretical studies of the aluminum-water clusters $Al(H_2O)_n$ and their ions $[Al(H_2O)_n]^+$. Hidekazu Watanabe, Masaharu Aoki, Suehiro Iwata, Bull.Chem.Soc.Japan, 66 (1993) 3245-3252
- 105 Theoretical Assignment of the vibronic bands in the photoelectron spectra of N_2 below 30 eV. Miyabi Hiyama and Suehiro Iwata, Chem.Phys.Letters, 211 (1993) 319-327
- 104 Electronic structure and reactivity of $Mg^+(H_2O)_n$ cluster ions. Kiyohiko Fuke, Fuminori Misaizu, Masaomi Sanekata, Keizo Tsukamoto and Suehiro Iwata, Z.Phys. D, 26 (1993) 180-183
- 103 The Photodissociation dynamics of Ar_3^+ . Tsutomu Ikegami, Tamotsu Kondow and Suehiro Iwata, J.Chem.Phys. 99 (1993) 3588-3596
- 102 Assignment of the Photoelectron Spectrum of HCl above 20 eV. Miyabi Hiyama and Suehiro Iwata, Chem.Phys.Letters, 210 (1993) 187-192
- 101 The geometric and electronic structures of Ar_n^+ (n = 3 - 27). Tsutomu Ikegami, Tamotsu Kondow and Suehiro Iwata , J.Chem.Phys. 98 (1993) 3038-3048
- 100 Photodissociation of size-selected $Mg^+(H_2O)_n$ ions for n = 1 and 2. Fuminori Misaizu, Masaomi Sanekata, Keizo Tsukamoto, Kiyohiko Fuke and Suehiro Iwata, J.Phys.Chem. 96 (1992) 8259-8264
- 99 Theoretical study of Aluminum-Sodium bimetallic cluseters. I: Geometrical and electronic structures of Al_nNa (n=1 - 4), Hidenori Matsuzawa, Toshiyuki Hanawa, Kazunori Suzuki and Suehiro Iwata, Bull.Chem.Soc.Jpn. 65 (1992) 2578-2588

- 98 Electronic spectra of p-dicyanobenzene (p-DCNB), p-DCNB-H₂O complex, and p-DCNB dimer in a supersonic jet. Keiko Fujita, Takashige Fujiwara, Kentaro Matsunaga, Fuminobu Ono, Atsushi Nakajima, Hironao Watanabe, Tomohisa Koguchi, Isamu Suzuki, Hidenori Matsuzawa, Suehiro Iwata and Koji Kaya, J.Phys.Chem. 96 (1992) 10693-10697
- 97 Theoretical studies of new radicals SiNNH and SiCOH. Kangnian Fan and Suehiro Iwata, Chem.Phys.Letters, 195 (1992) 475-481
- 96 The excimer emission spectra and the interaction potential energy of the ground and excited states of He and alkali-metal ion systems. Miyabi Hiyama, Shinkoh Nanbu and Suehiro Iwata, Chem.Phys.Letters, 192 (1992) 443-450
- 95 Ab initio study of the infrared absorption bands and their intensities for ethylene-halogen and amine-halogen complexes. Hidenori Matsuzawa and Suehiro Iwata, Chem. Phys. 163 (1992) 297-305
- 94 Theoretical study of the photodissociation cross sections and the photodissociation dynamics of HOCl. Shinkoh Nanbu and Suehiro Iwata, J. Phys. Chem., 96 (1992) 2103-2111
- 93 Ab initio Study of the Potential Energy Surfaces for the Radiative Association Reaction C⁺ + H₂ -> CH₂⁺ + hν. Agee Ozeki and Suehiro Iwata, "Chemistry and Spectroscopy in Interstellar Molecules", Ed. by D.K. Bohme, E. Herbst, N. Kaifu and S. Saito, University of Tokyo Press, Tokyo. (1992) 179-181,
- 92 Theoretical study of the three isomers of the SiNO radical. Kangnian Fan and Suehiro Iwata, Chem.Phys.Letters, 189 (1992) 401-407
- 91 Ab initio studies of the low-lying states of BeO. Jun Irisawa and Suehiro Iwata, Theor.chim.Acta, 81 (1992) 223-235
- 90 Optogalvanic spectrum of the CO L' ¹Π - B¹Σ⁺(v=0) band and electronic structure of the L' ¹Π state. Sigeyuki Sekine, Suehiro Iwata and Chiaki Hirose, Chem.Phys.Letters, 180 (1991) 173-178
- 89 Correlation of Electron Density and Spin-Exchange interaction in Dimeric Copper(II) Formates Acetates and Silanecarboxylates. Michinari Yamanaka, Hidehiro Uekusa, Shigeru Ohba, Yoshihiko Saito, Suehiro Iwata, Michinobu Kato, Tadashi Tokii, Yoneichiro Muto and Omar W. Steward, Acta Cryst. B47 (1991) 344-355
- 88 Ab initio calculations of the dipole moment and frequency-dependent polarizability for silicon monoxide and its anion. Toshihiro Inoue and Suehiro Iwata J.Molec.Struc. (THEOCHEM), 243 (1991) 147-162
- 87 Theoretical studies of vacuum ultraviolet emission spectra of NeLi⁺ and ArLi⁺. Suehiro Iwata, Shinkoh Nanbu and Hideki Kitajima, J. Chem. Phys. 94 (1991) 3707-3714
- 86 An MCSCF study of the low-lying states of C₂H⁺. Kenro Hashimoto, Suehiro Iwata, Yoshihiro Osamura, Chem. Phys. Letters, 174 (1990) 649-654
- 85 Photodissociation of Ar₃⁺ cluster ion. Takashi Nagata, Jun Hirokawa, Tsutomu Ikegami, Tamotsu Kondow and Suehiro Iwata, Chem. Phys. Letters, 171 (1990) 433-438
- 84 Method of frequency-dependent hyperpolarizability calculation from large-scale CI matrices. Toshihiro Inoue and Suehiro Iwata, Chem. Phys. letters, 167 (1990) 566-570
- 83 Molecular orbital study on the mechanism of oxidation of a beryllium atom in acidic solution, Kenro Hashimoto, Nobuyuki Yoda, Yoshihiro Osamura and Suehiro Iwata, J. Amer. Chem. Soc., 112 (1990) 7189-7196
- 82 Induced infrared absorption bands of ethylene adsorbed on mordenites: Experimental and theoretical studies of electron-donor-acceptor interactions. Hidenori Matsuzawa, Hiroshi Yamashita, Mastoki Ito and Suehiro Iwata, Chem. Phys., 147 (1990) 77-83
- 81 Ab initio self-consistent-field molecular orbital study on the hydration of three oxidation states of beryllium in aqueous solution. Kenro Hashimoto and Suehiro Iwata, J. Phys. Chem., 93 (1989) 2165-2169
- 80 Second-order Jahn-Teller effect of cyclobutadiene in low-lying states. An MCSCF study. Kensuke Nakamura, Yoshihiro Osamura and Suehiro Iwata, Chem. Phys., 136 (1989) 67-77
- 79 Theoretical study of the photoabsorption cross sections of HOCl and HOF. Shinkoh Nambu, Kazuto Nakata and Suehiro Iwata, Chem. Phys., 135 (1989) 75-83
- 78 A theoretical study of the photodissociation of acetylene in its lowest excited singlet state., Yoshihiro Osamura, Fujiko Mitsuhashi and Suehiro Iwata, Chem. Phys. Letters, 164 (1989) 205-

- 77 Promotion of the proton transfer reaction by the intermolecular stretching mode: Application of the two-dimensional finite element method to the nuclear Schrodinger equation. Nobuyuki Sato and Suehiro Iwata, *J. Chem. Phys.*, 89 (1988) 2932 - 2937
- 76 Theoretical emission spectra of NeAl^+ and ArAl^+ in the vacuum ultraviolet region. Nobuyuki Sato, Sinko Nanbu and Suehiro Iwata, *Chem. Phys. Letters* 146 (1988) 275-279
- 75 Application of the higher order finite element method to one-dimensional Schrodinger equation. Toshiyasu Kimura, Nobuyuki Sato and Suehiro Iwata, *J. Comput. Chem.*, 9 (1988) 827-835
- 74 Application of finite element-method to the two-dimensional Schrodinger equation., Nobuyuki Sato and Suehiro Iwata, *J. Comput. Chem.*, 9 (1988) 222-231
- 73 The high-resolution photoabsorption spectra of PH_3 , PF_3 , PCl_3 and PBr_3 in the XUV region., Eiji Ishiguro, Suehiro Iwata, Akira Mikuni, Yoshio Suzuki, Hideto Kanamori and Taizo Sasaki, *J. Phys. B.*, 20 (1987) 4725-4739
- 72 Theoretical study of hydrated Be^{2+} ions. Kenro Hashimoto, Nobuyuki Yoda and Suehiro Iwata, *Chem. Phys.*, 116 (1987) 193-202
- 71 Ab initio study of structure and stability of beryllium compounds. Kenro Hashimoto, Yoshihiro Osamura and Suehiro Iwata, *J. Molec. Struct. THEOCHEM*, 152 (1987) 101-117
- 70 Basis-set dependence of theoretical deformation density in NO_2^- , Tomoaki Kikkawa, Shigeru Ohba, Yoshihiro Saito, Shinichi Kamata and Suehiro Iwata, *Acta Cryst.*, B43 (1987) 83-85
- 69 水素で橋かけしたベリリウム化合物の構造に関する理論的研究, Kenro Hashimoto, Yoshihiro Osamura and Suehiro Iwata, *日本化学会誌*, (1986) 1377-1383
- 68 非経験的分子軌道法による原子の酸化状態の研究, Keiko Takano, Haruo Hosoya and Suehiro Iwata, *日本化学会誌*, (1986) 1395-1403
- 67 Quantum chemical interpretation of oxidation number with ab initio molecular orbital wavefunctions., Keiko Takano, Haruo Hosoya and Suehiro Iwata, "Applied Quantum Chemistry", Ed. by V. H. Smith, Reidel, (1986) 375 – 393
- 66 Ab initio studies on the vacuum ultraviolet (VUV) excimer emission spectra of NeB^+ and ArB^+ ., Suehiro Iwata and Nobuyuki Sato, *J. Chem. Phys.* 83 (1985) 2346 - 2351
- 65 The CI calculation of the frequency-dependent polarizability and some optical properties for N_2 and O_2 , Toshihiro Inoue, Shinji Matsushima and Suehiro Iwata, *Mol. Phys.* 56 (1985) 1097-1115
- 64 Photon energy dependence of the electron spectra of BF_3 near the boron K ionisation energy, Hideo Kanamori, Suehiro Iwata, Akira Mikuni and Taizo Sasaki, *J.Phys.B*17 (1984) 3887 - 3900
- 63 An MCSCF study of the low-lying states of trans-butadiene, Mutsumi Aoyagi, Yoshihiro Osamura and Suehiro Iwata, *J. Chem.Phys.* 83 (1984) 1140 - 1148 x
- 62 Quantum chemical interpretation of oxidation number applied to carbon and oxygen compounds. Numerical analysis of the electron distribution with ab initio molecular orbital wave functions, Keiko Takano, Haruo Hosoya, and Suehiro Iwata, *J. Am.Chem.Soc.* 106 (1984) 2787- 2792
- 61 Excitation and dispersed fluorescence spectra of ${}^1\text{B}_2(\text{V}) - {}^1\Sigma_g^+(\text{X})$ transition of jet-cooled CS_2 . Hiroshi Kasahara, Naohiko Mikami, Mitsuo Ito, Suehiro Iwata and Isao Suzuki, *Chem.Phys.* 86 (1984) 173 - 188
- 60 Fluorescence cross sections and electronic transition moments for the $\text{A}^2\Sigma^+ \rightarrow \text{X}^2\Pi$ transition in HCl^+ by photoionization.. Comparison with the ab initio calculations. Toshio Ibuki, Nobuyuki Sato, Suehiro Iwata, *J.Chem.Phys.* 79 (1983) 4805 - 4810
- 59 Direct calculation of the frequency-dependent polarizability from a Cl matrix. Suehiro Iwata, *Chem.Phys.Letters* 102 (1983) 544 - 549
- 58 Electronic and molecular structure of the water dimer cation. A theoretical study., Kennji Sato, Rhinji Tomoda, Katsumi Kimura and Suehiro Iwata, *Chem.Phys.Letters*, 95 (1983) 579- 583
- 57 Photoelectron angular distribution and assignments of photoelectron spectra of nitrogen dioxide, nitromethane and nitrobenzene, Shunji Katsumata, Haruo Shiromaru, Kazuhiro Mitani, Suehiro Iwata, Katsumi Kimura, *Chem.Phys.* 69 (1982) 423 - 431
- 56 Analysis of the oxidation state and oxidation number by ab initio molecular orbital calculations: chlorine and sulfur compounds. Keiko Takano, Haruo Hosoya and Suehiro Iwata, *J.Am.Chem.Soc.* 104 (1982) 3998 - 4005

- 55 Photoionization mass spectrometric study of acetylene in VUV region. Tatsuya Hayaishi, Suehiro Iwata M.Sasanuma, Eiji Ishiguro, Y.Moroka, Y.Iida and Masatoshi Nakamura, J.Phys.B 15 (1982) 79 - 92
- 54 The boron K photoabsorption spectra of BF_3 , BCl_3 and BBr_3 . Eiji Ishiguro, Suehiro Iwata, Yoshio Suzuki, Akira Mikuni, Taizo Sasaki, J.Phys. 15 (1982) 1841 - 1854
- 53 The ab initio potential energy surfaces of some low-lying states of acetylene. Okio Nomura and Suehiro Iwata, J.Chem.Phys. 74 (1981) 6830 - 6841
- 52 Valence type vacant orbitals for configuration interaction calculation., Suehiro Iwata, Chem.Phys.Letters 83 (1981) 134 - 138
- 51 Chlorine L absorption cross sections of gaseous HCl and Cl_2 . K.Ninomiya, Suehiro Iwata, Yoshio Suzuki, Akira Mikuni, Taizo Sasaki, J.Phys. B14 (1981) 1777 - 1790
- 50 Quantum chemistry literature database. Yoshihiro Osamura, Shinichi Yamabe, Fumio Hirota, Suehiro Iwata, Hiroshi Kashiwagi, Keiji Morokuma, M.Togashi, Shigeru Obara, Kiyoshi Tanaka and Kimio Ohno, J.Chem.Inform.Comp.Science, 21 (1981) 86 - 90
- 49 Double Breakdown of Koopmans' Theorem and Strong Correlation Satellites in the He II photoelectron spectrum of O_3 . Nobuhiro Kosugi, Haruo Kuroda and Suehiro Iwata, Chem. Phys. 58 (1981) 267 - 273
- 48 Ab initio Studies of the Hydrogen Atom Addition to Ethylene, Okio Nomura and Suehiro Iwata, Bull. Chem. Soc. Jpn. 53 (1980) 61 - 67
- 47 An Alternative Way to Analyze the Electron Distribution in Ab initio Calculations., Suehiro Iwata, Chem. Phys. Letters 69 (1980) 305 - 312
- 46 QCLDB : Quantum Chemistry Literature Data Base. A trial. Yoshihiro Osamura, Shinichi Yamabe, Fumio Hirota, Suehiro Iwata, Hiroshi Kashiwagi, Keiji Morokuma, M.Togashi, Shigeru Obara, Kiyoshi Tanaka, and Kimio Ohno, Int.J.Quant.Chem. 18 (1980) 393 - 396
- 45 Active Reaction Subsystem CI Studies of Peroxy Free Radicals. Aminoperoxy radical(H_2NO_2). Kizashi Yamaguchi and Suehiro Iwata, Chem.Phys. Letters 76 (1980) 375 - 379
- 44 Ab initio UHF and UHF NO CI approaches for Quasi-Degenerate system: Methyleno peroxide(CH_2OO). Kizashi Yamaguchi, Satoshi Yabushita, Takayuki Fueno, Shigeki Kato, Keiji Morokuma and Suehiro Iwata, Chem.Phys.Letters 71 (1980) 563 - 568
- 43 Magnetic Field Effects on the Fluorescence of Methylglyoxal. Kazuhito Hashimoto, Saburo Nagakura, Junko Nakamura and Suehiro Iwata, Chem.Phys. Letters 74 (1980) 228 - 231
- 42 Semiempirical MO study on the Abnormal bond orders of large Networks of highly Branched Polyenes. Tomoko Kanazawa, Suehiro Iwata and Haruo Hosoya, Int.J. Quant.Chem. 15 (1979) 243 - 257
- 41 Potential Energy Curves of Several Excited States of the Ne_2^* excimer: Assignment of the transient absorption spectra of the excimer, Suehiro Iwata, Chem. Phys. 37 (1979) 251 - 257
- 40 Breakdown of Koopmans' Theorem and Strong Shake-up Bands in the Valence Shell Region of N_2 photoelectron spectra. Nobuhiro Kosugi, Haruo Kuroda and Suehiro Iwata, Chem.Phys. 39 (1979) 337 - 349
- 39 Potential energy curves of Low-Lying states of HNO. Okio Nomura and Suehiro Iwata, Chem. Phys. Letters, 66 (1979) 523 - 526
- 38 Transannular interaction in the excited triplet states of [2,2] paracyclophane and related compounds. Shun-ichi Ishikawa, Junko Nakamura, Suehiro Iwata, Minoru Sumitani, Saburo Nagakura, Yoshiteru Sakata and Soichi Misumi, Bull. Chem. Soc. Jpn. 52 (1979) 1346-1350
- 37 Theoretical Studies on Inner Shell Excitations of CO, N_2 and C_2H_2 ., Suehiro Iwata, Nobuhiro Kosugi and Okio Nomura, Jpn.J.App.Phys. S17 (1978) 109 -111
- 36 One-center Two Electron Repulsion Parameters in the π and all-valence Semi-Empirical theories, .Suehiro Iwata, Chem.Phys.Letters, 57 (1978) 247 - 252
- 35 Electronic Structures and Spectra of Aminoacetophenones and Related Compounds, Ryoichi Nakagaki, Saburo Nagakura, Takayoshi Kobayashi and Suehiro Iwata, Bull.Chem.Soc.Jpn. 51 (1978) 2867 -2872
- 34 Ab initio studies of β -decay in OHT, NH_2T , CH_3T and $^{14}\text{CH}_4$, .Shigeru Ikuta, Suehiro Iwata and Masashi Imamura, J.Chem.Phys. 66 (1977) 4671 - 4676
- 33 Molecular orbital studies of hydrogen bonds. X. The ground and low-lying excited states of formic

- acid dimer., Suehiro Iwata and Keiji Morokuma, *Theor. chim. Acta* 44 (1977) 323 -
- 32 Electronic Absorption Bandwidths of Negative Ions of Aromatic Hydrocarbons. Tsutomu Watanabe, Tadamasa Shida and Suehiro Iwata, *Chem.Phys.* 13 (1976) 65-
- 31 Nonclassical Therms in the true Effective Valence Shell Hamiltonian:A Second Qnanzited Formalism., Suehiro Iwata, Karl F. Freed, *J.Chem.Phys.* 65 (1976) 1071 - 1088
- 30 Analysis of Exact Valence Shell Hamiltonian: Nonclassical Terms and Molecular Based Parameters, Suehiro Iwata and Karl F. Freed, *Chem.Phys. Letters* 38 (1976) 425 - 431
- 29 Molecular Orbital Studies of Hydrogen Bonds. VI. Origin of red shift of $\pi-\pi^*$ transitions. trans-Acrolein-Water complex., Suehiro Iwata, Keiji Morokuma, *J.Am. Chem.Soc.* 97 (1975) 966 - 970
- 28 Solution of Large Configuration Mixing Matrices Arising in Partitioning Technique and applications to the generalized eigenvalue problem, Suehiro Iwata and Karl F. Freed, *Chem.Phys.* 11 (1975) 433 - 440
- 27 Theoretical Study of the Photoetector Intensities and Angular Distributions. Suehiro Iwata and Saburo Nagakura, *Mol.Phys.* 27 (1974) 425 - 440
- 26 Multi-Configuration Electron-Hole Potential Method for Excited States, Suehiro Iwata and Keiji Morokuma, *Theor.Chem.Acta* 33 (1974) 285 - 297
- 25 Ab initio Evaluation of Correlation Contributions to the True π -electron hamiltonian: Ethylene. Suehiro Iwata and Karl F.Freed, *J.Chem.Phys.* 61 (1974) 1500 - 1509
- 24 Ab inito calculation of the π -Electron hamiltonian: Singlet-Triplet separation, Suehiro Iwata, and Karl F.Freed, *Chem.Phys.Leetters* 28 (1974) 176 - 178
- 23 Electronic Absorption Spectra of Ion-Radicals and Their Molecular Orbital Interpretation. IV. Anion Radicals of aromatic and Unsaturated aliphatic carbonyl compounds. Tadamasa Shida, Suehiro Iwata and Masashi Imamura, *J.Phys.Chem.* 78 (1974) 741 - 748
- 22 Molecular Orbital Studies of Hydrogen Bonds. V. Analysis of the hydrogen Bond Energy Between Lower Excited States of H_2CO and H_2O . Suehiro Iwata and Keiji Morokuma, *J.Am.Chem.Soc.* 95 (1973) 7563 - 7575
- 21 The Triplet-Triplet Absorption Spectra of Electron-Acceptor complexes. Satoru Matsumoto, Saburo Nagakura, Suehiro Iwata and Junko Nakamura, *Mol.Phys.* 26 (1973) 1465 -1474
- 20 Molecular Orbital Studies of Hydrogen Bonds. IV. Hydrogen Bonds in Excited States of H_2CO with H_2O . Suehiro Iwata and Keiji Morokuma, *Chem.Phys.Letters* 19 (1973) 94 - 98
- 19 Electronic Spectra of ion Radicals and their Molecular Orbital Interpretation. III. Aromatic hydrocarbons.Tadamasa Shida and Suehiro Iwata, *J.Am.Chem.Soc.* 95 (1973)_3473 - 3483
- 18 Electronic Spectra and Electronic Structures of [2,2] paracyclophane and related compounds,. Suehiro Iwata, Kiyohiko Fuke, Michiko Sasaki, Saburo Nagakura, Tetsuo Otsubo and Soichi Misumi, *J. Molec.Spectr.* 46 (1973) 1 - 15
- 17 The Electronic Absorption Spectra and Electronic Structures of Aromatic Azides, Nitrenes and Diazonium Ions. I. Hiroshi Kashiwagi, Suehiro Iwata, Y.Yamaoka, Saburo Nagakura, *Bull.Chem.Soc. Jpn.* 46 (1973) 417 -
- 16 π Electron Structures of Aromatic Hydrocarbons in their low-lying triplet states., Hiroshi Kashiwagi, Suehiro Iwata and Saburo Nagakura, *Bull.Chem.Soc.Jpn.* 46 (1973) 3289 - 3290
- 15 Electronic Absorption Spectra of Excess Electrons in Molecular Aggregates. II..Solvated electrons. Tadamasa Shida, Suehiro Iwata, Tsutomu Watanabe, *J.Phys.Chem.* 76 (1972) 3691 - 3694
- 14 Electronic absorption spectra of excess electrons in molecular aggregates. I.Trapped electrons in γ -irradiated amorphous solids at 77K. Tadamasa Shida, Suehiro Iwata, and Tsutomu Watanabe, *J.Phys.Chem.* 76 (1972) 3683 - 3691
- 13 Extended Hartree-Fock Theory for Excited States. Keiji Morokuma and Suehiro Iwata, *Chem.Phys.Letters*, 16 (1972) 192-
- 12 Absorption spectra of dianthracene dimer anion. Tadamasa Shida and Suehiro Iwata, *J.Chem.Phys.* 56 2858 - 2864 (1972)
- 11 The triplet-triplet absorption spectra observed for some tetracyanobenzene complexes. Satoru Matsumoto, Suehiro Iwata, Junko Nakamura and Saburo Nagakura, *Chem.Phys.Letters*, 13 (1972) 463 -
- 10 Electronic spectra of ion radicals and their molecular orbital interpretation. I. Aromatic nitro-

- substituted Anion-Radicals. Tadamasa Shida and Suehiro Iwata, J. Phys. Chem. 75 (1971) 2591 -
- 9 Charge-transfer complexes of maleic anhydride and dichloromaleic anhydride with various aromatic compounds. Tadayoshi Kobayashi, Suehiro Iwata and Saburo Nagakura, Bull.Chem.Soc.Jpn. 43 (1970) 713 -
- 8 ESR spectra of the charge-transfer triplet state of some molecular complexes. Hisashi Hayashi, Suehiro Iwata and Saburo Nagakura, J.Chem.Phys. 50 (1969) 993 -
- 7 Absorption and emission spectra of 1,2,4,5-tetracyanobenzene - naphthalene complex crystal. Suehiro Iwata, Jiro Tanaka and Saburo Nagakura, J.Am.Chem.Soc. 89 (1967) 2813 - 2819
- 6 ESR of the charge-transfer triplet state of durene-tetracyanobenzene complex. Hisaharu Hayashi, Saburo Nagakura and Suehiro Iwata, Mol.Phys. 13 (1967) 489-490
- 5 Charge-Transfer triplet state of molecular complexes. Phosphorescence of the charge-transfer triplet states of some molecular complexes. Suehiro Iwata, Jiro Tanaka and Saburo Nagakura, J.Chem.Phys. 47 (1967) 2203 - 2209
- 4 Charge-Transfer triplet state of molecular complexes. Phosphorescence of the charge-transfer triplet states of some molecular complexes. Suehiro Iwata, Jiro Tanaka and Saburo Nagakura, "Triplet State", Cambridge Press, (1967) 433-438
- 3 Molecular complexes between 1,2,4,5-tetracyanobenzene and some aromatic electron donors., Suehiro Iwata, Jiro Tanaka and Saburo Nagakura, J. Am.Chem.Soc. 88 (1966) 894 - 902
- 2 Charge-transfer complexes of trinitrobenzene with tetramethyl-p-phenylenediamine and p-Dimethoxybenzene. Suehiro Iwata, Hiroshi Tsubomura and Saburo Nagakura, Bull.Chem.Soc.Jpn. 37 (1964) 1506-151
- 1 Microwave spectrum of s-trioxane. Takeshi Oka, K. Tsuchiya, Suehiro, Iwata and Yonezo Morino, Bull.Chem.Soc. Jpn. 37 (1964) 374

総合報告

- 31 「RAE2008 に向けて:UK における研究評価事業、翻訳『下院科学技術委員会 再審議』『RAE2008 申請の手引き』の解題と英国調査報告」, 岩田末廣、大学評価・学位授与機構紀要「大学評価・学位研究」5 (2007) 136-159
- 30 「RAE2001 から RAE2008 へ:『下院委員会報告』『ロバーツ報告』と『RAE2008』の解題」、岩田末廣、大学評価・学位授与機構紀要「大学評価・学位研究」, 3 (2005) 131-136
- 29 「大学評価・学位授与機構による試行評価に現れた工学系大学院の状況と課題」、徳田昌則、岩田末廣、工学教育、52 (2004) 50-55、
- 28 「英国の研究評価事業における評価部会の基準と作業手順—資料『RAE 文書 5/99』の解説」、岩田末廣、徳田昌則、大学評価・学位授与機構紀要「大学評価」、2 (2002) 57-61
- 27 「研究評価」、岩田末廣、実験化学講座第 6 版、基礎編 I, 丸善、(2003) 436-444
- 26 Electron correlation and Coulomb hole deduced from X-ray scattering intensities: Experimental and theoretical studies. Noboru Watanabe, Seiichiro Ten-no, Suehiro Iwata and Yasuo Udagawa, "REVIEWS IN MODERN QUANTUM CHEMISTRY. A CELEBRATION OF THE CONTRIBUTIONS OF R. G. PARR", Ed. by K. D. Sen, (2002) 553-576
- 25 ノーベル賞と分光学 II. 定量的量子化学計算理論の開拓と確立、岩田末廣、分光研究、50 (2001) 80-85
- 24 Electronic and geometric structures of water cluster complexes with a group 1 metal atom: Electron-hydrogen bond in the OH{e}HO structure. Suehiro Iwata and Takeshi Tsurusawa, Advances in Metal and Semiconductor Clusters, 5 (2001) 39-75
- 23 Structures, spectroscopies and reactions of atomic ions with water clusters, Kiyokazu Fuke, Kenro Hashimoto, Suehiro Iwata, Adv. Chem.Phys., 110 (1999) 431.
- 22 化学結合論・量子化学・計算化学、岩田末廣、学術月報 52 (1999) 570-576
- 21 定量的量子化学計算理論の開拓と確立—ポープル教授とコーン教授の業績—、岩田末廣、現代化学、(1998) 20

- 20 量子化学計算はどこまで信頼できるか?、岩田末廣、化学と工業、48 (1995) 815-816
- 19 分子の光電子スペクトルとイオン状態、木村克美、勝又春次、阿知波洋次、山崎トモ子、岩田末廣、学会出版センター (1995)
- 18 量子化学、岩田末廣、”量子化学”、濱田嘉昭・朽津耕三編集、放送大学教育振興会 (1993)
- 17 化学結合の量子化学、岩田末廣、”大学院物理化学”、妹尾学・広田襄・田隅三生・岩澤康祐編集、講談社 (1992)
- 16 ワークステーションを利用した計算化学、岩田末廣、南部伸孝、入沢潤、現代化学 (1990) (11月) 18-22
- 15 計算化学による光化学反応の解析、岩田末廣、南部伸孝、分光研究、39 (1990) 303-316
- 14 分子間力の量子化学、岩田末廣、”分子シミュレーション”、岡田勲・大澤映二編集、海文堂 (1989)
- 13 クラスターの量子化学：分子からのアプローチ、岩田末廣、数理科学、(1989)
- 12 量子化学計算による電子密度解析、岩田末廣、日本結晶学会誌、30 (1988) 129-134
- 11 シュレディンガー方程式の数値解法、佐藤信行、岩田末廣、Bit, 19 (1987) 1761-1768
- 10 分子のシュレディンガー方程式を解く — 電子計算機による分子の構造と性質の予測 —、岩田末廣、現代化学、(1984) 54-60
- 9 Reliability of ab initio calculations, Suehiro Iwata, “Quantum Chemistry Literature Data Base”, Ed. by Kimio. Ohno, Haruo.Hosoya, North Holand, (1982)
- 8 分子分光学と量子化学 — メチレン(CH_2)を例として —、岩田末廣、化学、37 (1982) 29-31
- 7 量子化学計算の分子分光学への応用 II、岩田末廣、分光研究、30 (1981) 77-92
- 6 量子化学計算の分子分光学への応用 I、岩田末廣、分光研究、30 (1981) 3-16
- 5 Handbook of HeI photoelectron spectra of fundamental organic molecules, Katsumi Kimura, Shunji Katsumata, Y.Achiba, T.Yamazaki, Suehiro.Iwata, Jpn. Scientific Soc. Press, Tokyo, (1980)
- 4 原子価電子の有効ハミルトニアン、岩田末廣、化学の領域、30 (1976) 41-49
- 3 シンクロtron放射の分子分光への応用 — 主として N_2 と SF_6 について —、岩田末廣、科学、44, (1974) 620-627
- 2 Molecular interactions in ground and excited states, Keiji Morokuma, Suehiro.Iwata, W.A.Lathan, 'The Worlds of Quantum Chemistry.', Ed.R.Daudel and B.Pullman, D.ReideI,Holland (1974)
- 1 発光X線スペクトルの化学結合効果、岩田末廣、日本結晶学会誌、11 (1969) 102-108,