

業績リスト 波田雅彦 2022年10月11日現在

1. Force in SCF Theories. MC SCF and Open-Shell RHF Theories,  
H. Nakatsuji, T. Hayakawa, Hada, *Chem. Phys. Letters*, **80**(1), 94-100 (1981).  
**DOI:** [https://doi.org/10.1016/0009-2614\(81\)80065-6](https://doi.org/10.1016/0009-2614(81)80065-6)
2. Force in SCF Theories. Test of New Method,  
H. Nakatsuji, K. Kanda, M. Hada, T. Yonezawa, *J. Chem. Phys.*, **77**(6), 3109-3122 (1982).  
**DOI:** <https://doi.org/10.1063/1.444234>
3. Force in SCF Theories. Combination with the Effective-Core Potential Method,  
H. Nakatsuji, M. Hada, T. Yonezawa, *Chem. Phys. Letters*, **95**(6), 573-578 (1983).  
**DOI:** [https://doi.org/10.1016/0009-2614\(83\)80358-3](https://doi.org/10.1016/0009-2614(83)80358-3)
4. Force in SCF Theories. First and Second Derivatives of the Potential Energy Hypersurface of Chemical Reaction Systems,  
H. Nakatsuji, M. Hada, K. Kanda, T. Yonezawa, *Intern. J. Quantum Chem.*, **XXIII**, 387-397 (1983).  
**DOI:** <https://doi.org/10.1002/qua.560230207>
5. Reply to Commemt on 'Force in SCF Theories,  
H. Nakatsuji, K. Kanda, M. Hada, T. Yonezawa, *J. Chem. Phys.*, **79**(5), 2493-2495 (1983).  
**DOI:** [10.1063/1.446090](https://doi.org/10.1063/1.446090)
6. Interaction of the Hydrogen Molecule with the Palladium Atom. A Force Theoretic Study,  
H. Nakatsuji , M. Hada, *Croatica Chem. Acta*, **57**(6), 1371-1386 (1984).
7. Interaction of a Hydrogen Molecule with Palladium,  
H. Nakatsuji , M. Hada, *J. Am. Chem. Soc.*, **107**(26), 8264-8266 (1985).  
**DOI:** [https://doi.org/10.1016/0021-9517\(71\)90193-X](https://doi.org/10.1016/0021-9517(71)90193-X)
8. Theoretical Study on the Catalytic Activity of Palladium for the Hydrogenation of Acetylene.  
H. Nakatsuji, M. Hada, T. Yonezawa, *Surf. Sci.*, **185**, 319-342 (1987).  
**DOI:** [https://doi.org/10.1016/S0039-6028\(87\)80629-5](https://doi.org/10.1016/S0039-6028(87)80629-5)
9. Theoretical Study on the Chemisorption of a Hydrogen Molecule on Palladium,  
H. Nakatsuji, M. Hada, T. Yonezawa, *J. Am. Chem. Soc.*, **109**(7), 1902-1912 (1987).  
**DOI:** [10.1021/ja00241a003](https://doi.org/10.1021/ja00241a003)

10. Frozen Core and Virtual Orbitals in the MCSCF Theory,  
M. Hada, H. Yokono, H. Nakatsuji, *Chem. Phys. Letters*, **141**(4), 339-345 (1987).  
**DOI:** [https://doi.org/10.1016/0009-2614\(87\)85035-2](https://doi.org/10.1016/0009-2614(87)85035-2)
11. Ab Initio MO Study of the Reaction of Pentacoordinate Allylsilicates with Aldehydes,  
M. Kira, K. Sato, H. Sakurai, M. Hada, M. Izawa, J. Ushio, *Chem. Letters*, 387-390 (1991).  
**DOI:** <https://doi.org/10.1246/cl.1991.387>
12. Ab Initio MO Calculations of Model Molecules for Ribozyme Reaction Including an Mg<sup>2+</sup> Ion,  
Y. Mizukami, H. Nakatsuji, M. Hada, M. Sasaki, N. Sugimoto, *Chem. Letters*, 2119-2122 (1991).  
**DOI:** <https://doi.org/10.1246/cl.1991.2119>
13. Electronic Structures of Dative Metal-Metal Bonds: Ab Initio Molecular Orbital Calculations of  
(OC)<sub>5</sub>Os-M(CO)<sub>5</sub> (M = W, Cr) in Comparison with (OC)<sub>5</sub>M-M(CO)<sub>5</sub> (M = Re, Mn),  
H. Nakatsuji, M. Hada, A. Kawashima, *Inorg. Chem.*, **31**(10), 1740-1744 (1992).  
**DOI:** [10.1021/ic00036a004](https://doi.org/10.1021/ic00036a004)
14. Does the Schrock-Type Metal-Silylene Complex Exist?,  
H. Nakatsuji, M. Hada, K. Kondo, *Chem. Phys. Letters*, **196**(5), 404-409 (1992).  
**DOI:** [https://doi.org/10.1016/0009-2614\(92\)85711-I](https://doi.org/10.1016/0009-2614(92)85711-I)
15. Theoretical study on the methane activation reactions by Pt, Pt<sup>+</sup>, and Pt<sup>-</sup> atoms,  
M. Hada, H. Nakatsuji, H. Nakai, S. Gyobu, S. Miki, *J. Mol. Struct. (THEOCHEM)*, **281**, 207-212 (1993).  
**DOI:** [https://doi.org/10.1016/0166-1280\(93\)87076-P](https://doi.org/10.1016/0166-1280(93)87076-P)
16. High Coordinate Germanium and Tin Complexes in the Allylation Reactions of Aldehydes,  
M. Hada, H. Nakatsuji, J. Ushio, M. Izawa, H. Yokono, *Organometallics*, **12**(9), 3398-3404 (1993).  
**DOI:** [10.1021/om00033a008](https://doi.org/10.1021/om00033a008)
17. Theoretical Study on the Molecular and Dissociative Adsorptions of H<sub>2</sub> on a ZrO<sub>2</sub> Surface,  
H. Nakatsuji, M. Hada, H. Ogawa, K. Nagata, K. Domen, *J. Phys. Chem.*, **98**(46), 11840-11845 (1994).
18. Theoretical Study on the Reaction Mechanism and Regioselectivity of Silastannation of Acetylenes with a  
Palladium Catalyst,  
M. Hada, Y. Tanaka, M. Ito, M. Murakami, H. Amii, Y. Ito, H. Nakatsuji, *J. Am. Chem. Soc.*, **116**(19),  
8754-8765 (1994).
19. Theoretical Study on the Ground and Excited States of the Chromate Anion CrO<sub>4</sub><sup>2-</sup>,  
S. Jitsuhiko, H. Nakai, M. Hada, H. Nakatsuji, *J. Chem. Phys.*, **101**(2), 1029-1036 (1994).

**DOI:** <https://doi.org/10.1063/1.467801>

20. Spin-Orbit Effect on the Magnetic Shielding Constant using the ab-initio UHF Method,  
H. Nakatsuji, H. Takashima, M. Hada, *Chem. Phys. Lett.*, **233**(1-3), 95-101 (1995).
21. Spin-orbit Effect on the Magnetic Shielding Constant using the ab initio UHF Method. Gallium and Indium Tetrahalides,  
H. Takashima, M. Hada, H. Nakatsuji, *Chem. Phys. Lett.*, **235**(1,2), 13-16 (1995).  
**DOI:** [https://doi.org/10.1016/0009-2614\(94\)01409-O](https://doi.org/10.1016/0009-2614(94)01409-O)
22. Theoretical Study on Metal NMR Chemical Shifts. Arsenic and Antimony Compounds,  
H. Takashima, M. Hada, and H. Nakatsuji, *J. Phys. Chem.*, **99**(20), 7951-7957 (1995).  
**DOI:** [10.1021/j100020a017](https://doi.org/10.1021/j100020a017)
23. Theoretical Study of the Transition Energies of the Visible Absorption Spectra of  $[\text{RhCl}_6]$  and  $[\text{RhCl}_5(\text{H}_2\text{O})]^{2-}$  Complexes in Aqueous Solution.  
K. Endo, M. Saikawa, M. Sugimoto, M. Hada, H. Nakatsuji, *Bull. Chem. Soc. Jpn.*, **68**, 1601-1605 (1995).  
**DOI:** <https://doi.org/10.1246/bcsj.68.1601>
24. Theoretical Study on the Chemisorption and the Surface Reaction of  $\text{HCOOH}$  on a  $\text{MgO}(001)$  Surface,  
H. Nakatsuji, M. Yoshimoto, M. Hada, K. Domen, C. Hirose, *Surf. Sci.*, **336**, 232-244 (1995).  
**DOI:** [https://doi.org/10.1016/0039-6028\(95\)00484-X](https://doi.org/10.1016/0039-6028(95)00484-X)
25. Spin-Orbit Effect on the Magnetic Shielding Constant using the ab-initio UHF method: Silicon Tetrahalides,  
H. Nakatsuji, T. Nakajima, M. Hada, H. Takashima, and S. Tanaka, *Chem. Phys. Letters*, **247**, 418-424 (1995).  
**DOI:** [https://doi.org/10.1016/S0009-2614\(95\)01266-4](https://doi.org/10.1016/S0009-2614(95)01266-4)
26. Theoretical Study on the Electronic Spectrum of  $\text{TcO}_4^-$ ,  
J. Hasegawa, K. Toyota, M. Hada, H. Nakai, H. Nakatsuji, *Theoret. Chim. Acta*, **92**, 351-359 (1995).  
**DOI:** <https://doi.org/10.1007/BF01114849>
27. Basis Set Dependence of Magnetic Shielding Constant Calculated by the Hartree-Fock / Finite Perturbation Method,  
T. Higashioji, M. Hada, M. Sugimoto, H. Nakatsuji, *Chem. Phys.*, **203**, 159-175 (1996).  
**DOI:** [https://doi.org/10.1016/0301-0104\(95\)00398-3](https://doi.org/10.1016/0301-0104(95)00398-3)
28. Topology of Density Difference and Force Analysis. I. Homopolar Bond Formation,  
S. J. Zheng, M. Hada, H. Nakatsuji, *Theoret. Chim. Acta*, **93**, 67-78 (1996).

**DOI:** <https://doi.org/10.1007/BF01113548>

29. Theoretical Study on the Excitation Spectrum and the Photofragmentation Reaction of Ni(CO)4,  
M. Hada, Y. Imai, M. Hidaka, H. Nakatsuji, *J. Chem. Phys.*, **103**(16), 6993-6998 (1995).  
**DOI:** <https://doi.org/10.1063/1.470325>
30. Excited and Ionized States of Free Base Porphin Studied by the Symmetry Adapted Cluster- Configuration Interaction (SAC-CI) Method,  
H. Nakatsuji, J. Hasegawa, M. Hada, *J. Chem. Phys.*, **104**(6), 2321-2329 (1996).  
**DOI:** <https://doi.org/10.1063/1.470927>
31. Ground and Excited States of Mg Porphin Studied by the SAC/SAC-CI Method,  
J. Hasegawa, M. Hada, M. Nonoguchi, H. Nakatsuji, *Chem. Phys. Letters*, **250**, 159-164(1996).  
**DOI:** [https://doi.org/10.1016/0009-2614\(95\)01406-3](https://doi.org/10.1016/0009-2614(95)01406-3)
32. Ground and Excited States of Oxyheme: SAC/SAC-CI Study,  
H. Nakatsuji, J. Hasegawa, H. Ueda, M. Hada, *Chem. Phys. Letters*, **250**, 379-386 (1996).  
**DOI:** [https://doi.org/10.1016/0009-2614\(96\)00033-4](https://doi.org/10.1016/0009-2614(96)00033-4)
33. Spin-Orbit Effect on the Magnetic Shielding Constant Using the Ab Initio UHF Method: Electronic mechanism in the Aluminium Compounds, AlX4- (X = H, F, Cl, Br, and I),  
H. Nakatsuji, M. Hada, T. Tejima, T. Nakajima, M. Sugimoto, *Chem. Phys. Letters*, **249**, 284-289 (1996).
34. Theoretical Study on Metal NMR Chemical Shifts. Electronic Mechanism of Xe Chemical Shift,  
S. Tanaka, M. Sugimoto, H. Takashima, M. Hada, H. Nakatsuji, *Bull. Chem. Soc. Japan*, **69**, 953-959 (1996).  
**DOI:** [https://doi.org/10.1016/0009-2614\(90\)85471-N](https://doi.org/10.1016/0009-2614(90)85471-N)
35. Cluster Quantum-Chemical MINDO/3 Study of the Nature of Hydroxyl Groups on a Calcium Oxide Surface,  
N. U. Zhanpeizov, H. Nakatsuji, M. Hada, *J. Mol. Catalysis A*, **112**, 63-69 (1996).  
**DOI:** [https://doi.org/10.1016/1381-1169\(96\)00132-X](https://doi.org/10.1016/1381-1169(96)00132-X)
36. CO and NO Adsorption on Copper-Containing Zeolite. Ab Initio Study,  
N. U. Zhanpeizov, H. Nakatsuji, M. Hada, H. Nakai, M. Anpo, *Catalysis Letters*, **42**, 173-176 (1996).  
**DOI:** <https://doi.org/10.1007/BF00810684>
37. Relativistic study of nuclear magnetic shielding constants: hydrogen halides,  
C. C. Ballard, M. Hada, H. Kaneko, H. Nakatsuji, *Chem. Phys. Letters*, **254**, 170-178 (1996).  
**DOI:** [https://doi.org/10.1016/0009-2614\(96\)00266-7](https://doi.org/10.1016/0009-2614(96)00266-7)

38. Relativistic Study on Nuclear Magnetic Shielding Constants: Mercury Dihalides,  
H. Nakatsuji, M. Hada, H. Kaneko, C. C. Ballard, *Chem. Phys. Letters*, **255**, 195-202 (1996).  
**DOI:** [https://doi.org/10.1016/0009-2614\(96\)00335-1](https://doi.org/10.1016/0009-2614(96)00335-1)
39. The Electronic Spectra of Ethylene,  
C. C. Ballard, M. Hada, H. Nakatsuji, *Bull. Chem. Soc. Japan*, **69**, 1901-1906 (1996).  
**DOI:** <https://doi.org/10.1246/bcsj.69.1901>
40. Ground and Excited States of Carboxyheme: a SAC/SAC-CI Study,  
N. Nakatsuji, Y. Tokita, J. Hasegawa, M. Hada, *Chem. Phys. Letters*, **256**, 220-228 (1996).  
**DOI:** [https://doi.org/10.1016/0009-2614\(96\)00906-2](https://doi.org/10.1016/0009-2614(96)00906-2)
41. Spin-Orbit Effect on the Magnetic Shielding Constant Using Ab Initio UHF Method: Tin Tetrahalides,  
H. Kaneko, M. Hada, T. Nakajima, H. Nakatsuji, *Chem. Phys. Letters*, **261**, 1-6 (1996).  
**DOI:** [https://doi.org/10.1016/0009-2614\(96\)00906-2](https://doi.org/10.1016/0009-2614(96)00906-2)
42. Relativistic Study of Nuclear Magnetic Shielding Constants: Tungsten hexahalides and Tungsten Tetraoxide,  
M. Hada, H. Kaneko, H. Nakatsuji, *Chem. Phys. Letters*, **261**, 7-12 (1996).  
**DOI:** [https://doi.org/10.1016/0009-2614\(96\)00905-0](https://doi.org/10.1016/0009-2614(96)00905-0)
43. Theoretical Study of the Chemisorption and Surface Reaction of HCOOH on a ZnO (101^0) Surface,  
H. Nakatsuji, M. Yoshimoto, Y. Umemura, S. Takagi, M. Hada, *J. Phys. Chem.*, **100**(2), 694-700 (1996).  
**DOI:** [10.1021/jp9504581](https://doi.org/10.1021/jp9504581)
44. Cluster Quantum-Chemical MINDO/3 Study of HCOOH Interactions with Nonpolar (101^0) Surface of ZnO,  
N. U. Zhanpeizov, H. Nakatsuji, M. Hada, M. Yoshimoto, *J. Mol. Catalysis A: Chemical*, **118**, 69-77 (1997).  
**DOI:** [https://doi.org/10.1016/S1381-1169\(96\)00382-2](https://doi.org/10.1016/S1381-1169(96)00382-2)
45. Relativistic theory of the magnetic shielding constant: a Dirac–Fock finite perturbation study,  
Y. Ishikawa, T. Nakajima, M. Hada, H. Nakatsuji, *Chem. Phys. Letters*, **283**, 119-124 (1998).  
**DOI:** [https://doi.org/10.1016/S0009-2614\(97\)01307-9](https://doi.org/10.1016/S0009-2614(97)01307-9)
46. First-Principles Molecular Dynamics Study of CO Adsorption on the Si(001) Surface,  
Y. Imamura, N. Matsui, T. Morikawa, M. Hada, T. Kubo, M. Nishijima, H. Nakatsuji, *Chem. Phys. Letters*, **287**, 131-136 (1998).  
**DOI:** [https://doi.org/10.1016/S0009-2614\(98\)00151-1](https://doi.org/10.1016/S0009-2614(98)00151-1)
47. Theoretical Study on the Decomposition of HCOOH on a ZnO (101~0) Surface,  
M. Yoshimoto, S. Takagi, Y. Umemura, M. Hada, H. Nakatsuji, *J. Cat.*, **173**, 55-63 (1998).

**DOI:** <https://doi.org/10.1006/jcat.1997.1889>

48. Self-Condensation Reaction of Lithium(Alkoxy)silylenoid: A Model Study by ab initio Calculation,  
Y. Tanaka, M. Hada, A. Kawachi, K. Tamao, H. Nakatsuji, *Organometallics*, **17**(21) 4573-4577 (1998).  
**DOI:** 10.1021/om980567c
49. Theoretical Study of the Excited States of Chlorin, Bacteriochlorin, Pheophytin a, and Chlorophyll a by the SAC/SAC-CI Method.  
J. Hasegawa, Y. Ozeki, K. Ohkawa, M. Hada, H. Nakatsuji, *J. Phys. Chem. B*, **102**(7), 1320-1326 (1998).  
**DOI:** 10.1021/jp972894o
50. Dirac-Fock Calculations of Magnetic Shielding Constants: Hydrogen Molecule and Hydrogen Halides,  
M. Hada, Y. Ishikawa, J. Nakatani, H. Nakatsuji, *Chem. Phys. Letters*, **310**, 342-346 (1999).  
**DOI:** [https://doi.org/10.1016/S0009-2614\(99\)00780-0](https://doi.org/10.1016/S0009-2614(99)00780-0)
51. Theoretical Study on the Decomposition of HCOOH on a MgO(100) Surface,  
M. Lintuluoto, H. Nakatsuji, M. Hada, K. Kanai, *Surface Sci.*, **429**, 133-142 (1999).  
**DOI:** [https://doi.org/10.1016/S0039-6028\(99\)00357-X](https://doi.org/10.1016/S0039-6028(99)00357-X)
52. Dirac-Fock Calculations of the Magnetic Shielding Constants of Protons and Heavy Nuclei in XH<sub>2</sub> (X = O, S, Se, and Te) -- A Comparison with Quasi-Relativistic calculations,  
M. Hada, R. Fukuda, H. Nakatsuji, *Chem. Phys. Letters*, **321**, 452-458 (2000).  
**DOI:** [https://doi.org/10.1016/S0009-2614\(00\)00375-4](https://doi.org/10.1016/S0009-2614(00)00375-4)
53. Electronic Excitation and Ionization Spectra of Cyclopentadiene: Revisit by the Symmetry-Adapted Cluster-Configuration Interaction Method,  
J. Wan, M. Ehara, M. Hada, H. Nakatsuji, *J. Phys. Chem.*, **113** (13), 5245-5252 (2000).  
**DOI:** 10.1063/1.1290004
54. Electronic Excitation Spectra of Furan and Pyrrole: Revisited by the Symmetry Adapted Cluster-Configuration Interaction method,  
J. Wan, M. Ehara, M. Hada, H. Nakatsuji, *J. Phys. Chem.*, **113** (18), 7853-7866 (2000).
55. Excited States of Four Hemes in c-type Cytochrome Subunit of Photosynthetic Reaction Center of Rhodopseudomonas viridis: SAC-CI Calculations,  
K. Ohkawa, M. Hada, H. Nakatsuji, *J. Porphyrins and Phthalocyanines*, **5**(3), 256-266 (2001).  
**DOI:** 10.1002/jpp.311.abs
56. Electronic Excitation and Ionization Spectra of Azabenzenes: I Pyridine, Rivisited by the Symmetry-Adapted Cluster Configuration Interaction Method,

J. Wan, M. Hada, M. Ehara, H. Nakatsuji, *J. Chem. Phys.*, **114** (12), 5117-5123 (2001).

57. Relativistic Effects and the Halogen Dependencies in the  $^{13}\text{C}$  Chemical Shifts of  $\text{CH}(4\text{-n})\text{I(n)}$ ,  $\text{CH}(4\text{-n})\text{Br(n)}$ ,  $\text{CCl}(4\text{-n})\text{I(n)}$ , and  $\text{CBr}(4\text{-n})\text{I(n)}$  ( $n=0\text{-}4$ ),

S. Fukawa, M. Hada, R. Fukuda, S. Tanaka, H. Nakatsuji, *J. Comp. Chem.*, **22**(5), 528-536 (2001).

**DOI:** 10.1002/1096-987X(20010415)22:53.0.CO;2-9

58. Quasi-Relativistic Study of  $^{199}\text{Hg}$  Nuclear Magnetic Shielding Constants of Dimethylmercury, Disilylmercury, and Digermylmercury,

J. Wan, R. Fukuda, M. Hada, H. Nakatsuji, *J. Phys. Chem. A*, **105**(1), 128-133 (2001).

59. Quasirelativistic Study of  $^{125}\text{Te}$  Nuclear Magnetic Shielding Constants and Chemical Shifts,

M. Hada, J. Wan, R. Fukuda, H. Nakatsuji, *J. Comp. Chem. (special issue for P. von R. Schleyer)*, **22**(13), 1502-1508 (2001).

**DOI:** <https://doi.org/10.1002/jcc.1103>

60. Effect of Ion-Exchanged Alkali Metal Cations on the Photolysis of 2-Pentanone Induced within ZSM-5 Zeolite Cavities: A Study of ab initio Molecular Orbital Calculations,

H. Yamashita, M. Nishimura, H. Bessho, S. Takada, T. Nakajima, M. Hada, H. Nakatsuji, M. Anpo, *Res. Chem. Intermed.*, **27**(1,2), 89-102 (2001).

**DOI:** <https://doi.org/10.1163/156856701745159>

61. Electronic Excitation Spectra of Thiophene Studied by Symmetry- Adapted Cluster Configuration Interaction Method,

J. Wan, M. Hada, M. Ehara, H. Nakatsuji, *J. Chem. Phys.*, **114**(2), 842-850 (2001).

**DOI:** 10.1063/1.1332118

62. Relativistic effects on magnetic circular dichroism studied by GUHF/SECI method,

Y. Honda, M. Hada, M. Ehara, H. Nakatsuji, J. Downing, J. Michl, *Chem. Phys. Lett.*, **355**, 219-225 (2002).

**DOI:** [https://doi.org/10.1016/S0009-2614\(02\)00125-2](https://doi.org/10.1016/S0009-2614(02)00125-2)

63. Ionized and excited states of ferrocene: Symmetry adapted cluster-configuration- interaction study,

K. Ishimura, M. Hada and H. Nakatsuji, *J. Chem. Phys.*, **117**, 6533-6537 (2002).

**DOI:** <https://doi.org/10.1063/1.1504709>

64. Excited and Ionized States of p-Benzoquinone and its Anion Radical: SAC-CI Theoretical Study,

Y. Honda, M. Hada, M. Ehara, H. Nakatsuji, *J. Phys. Chem. A*, **106**, 3838-3849 (2002).

**DOI:** 10.1021/jp013166a

65. Excited and ionized states of aniline: Symmetry adapted cluster configuration interaction theoretical study,  
Y. Honda, M. Hada, M. Ehara, H. Nakatsuji, *J. Chem. Phys.*, **117**, 2045-2052 (2002).  
**DOI:** <https://doi.org/10.1063/1.1487827>
66. Quasirelativistic theory for the magnetic shielding constant. I. Formulation of Douglas-Kroll-Hess transformation for the magnetic field and its application to atomic systems,  
R. Fukuda, M. Hada, H. Nakatsuji, *J. Chem. Phys.*, **118**, 1015-1026 (2003).  
**DOI:** <https://doi.org/10.1063/1.1528933>
67. Quasirelativistic theory for the magnetic shielding constant. II. Gauge-including atomic orbitals and applications to molecules,  
R. Fukuda, M. Hada, H. Nakatsuji, *J. Chem. Phys.*, **118**, 1027-1035 (2003).  
**DOI:** <https://doi.org/10.1063/1.1528934>
68. Quantum-Chemical Calculations for Paramagnetic  $^{13}\text{C}$  NMR Chemical Shifts of Iron-Bound Cyanide Ions of Iron Porphyrins in Ground and Low-Lying Excited States Containing Ferric  $(\text{d}_{xy})^2(\text{d}_{xz}, \text{yz})^3$  and  $(\text{d}_{xy})^1(\text{dxz}, \text{yz})^4$  Configurations,  
M. Hada, *J. Am. Chem. Soc.*, **126**(2), 486-487 (2004).  
**DOI:** [10.1021/ja038097n](https://doi.org/10.1021/ja038097n)
69. Experimental Study and Ab Initio Molecular Orbital Calculation on the Photolysis of n-butyrophenone included within the Alkali Metal Cation-Exchange ZSM-5 Zeolite,  
H. Yamashita, S. Takada, M. Hada, H. Nakatsuji, M. Anpo, *J. Photochem. Photobio. A: Chemistry*, **160**, 37-42 (2003).  
**DOI:** [https://doi.org/10.1016/S1010-6030\(03\)00218-1](https://doi.org/10.1016/S1010-6030(03)00218-1)
70. Nuclear Magnetic Shielding Constants of Halogens in X- and XO<sub>4</sub>-(X = F, Cl, Br, I) : Relativistic and Electron-Correlation Effects,  
H. Tanimura, M. Hada, *J. Comp. Chem. Japan*, **3**(4), 153-158 (2004).  
**DOI:** <https://doi.org/10.2477/jccj.3.153>
71. Theoretical studies on magnetic circular dichroism by the finite perturbation method with relativistic corrections,  
Y. Honda, M. Hada, M. Ehara, H. Nakatsuji, J. Michl, *J. Chem. Phys.*, **123**, 164113(1-9) (2005).  
**DOI:** [10.1063/1.2080027](https://doi.org/10.1063/1.2080027)
72. Relativistic configuration interaction and coupled cluster methods using four- component spinors: Magnetic shielding constants of HX and CH<sub>3</sub>X (X=F, Cl, Br, I),  
M. Kato, M. Hada, R. Fukuda, H. Nakatsuji, *Chem. Phys. Letters*, **408**, 150-156 (2005).

**DOI:** <https://doi.org/10.1016/j.cplett.2005.03.147>

73. Orientational Effect of Aryl Group on  $^{77}\text{Se}$  NMR Chemical Shifts: Experimental and Theoretical Investigations,  
W. Nakanishi, S. Hayashi, D. Shimizu, M. Hada, *Chemistry - A European Journal*, **12**, 3829-3846 (2006).  
**DOI:** <https://doi.org/10.1002/chem.200500927>
74. SAC and SAC-CI Calculations of Excitation and Circular Dichroism Spectra of Straight-Chain and Cyclic Dichalcogenes,  
J. Seino, Y. Honda, M. Hada, H. Nakatsuji, *J. Phys. Chem.*, **110**(33), 10053-10062 (2006).  
**DOI:** [10.1021/jp0627271](https://doi.org/10.1021/jp0627271)
75. Quantum Chemistry Literature Data Base II Bibliography of Ab Initio Calculations for 2005,  
N. Koga, T. Matsushita, K. Takano, K. Hashimoto, M. Hada, H. Hosoya, H. Matsuzawa, U. Nagashima, H. Wasada, S. Yamabe, *J. Comp. Chem. Japan*, **5**(5), 231-655 (2006).
76. Calculations of Frequency-Dependent Molecular Magnetizabilities with Quasi- Relativistic Time-Dependent Generalized Unrestricted Hartree-Fock Method,  
T. Yoshizawa, M. Hada, *J. Comp. Chem.*, **28**(4), 740-747 (2007).  
**DOI:** <https://doi.org/10.1002/jcc.20569>
77. How  $^{77}\text{Se}$  NMR Chemical Shifts Originate from Pre-alpha, alpha, beta, and gamma Effects: Interpretation Based on Molecular Orbital Theory,  
W. Nakanishi, S. Hayashi, M. Hada, *Chemistry A European J.*, **13**, 5282- 5293 (2007).  
**DOI:** <https://doi.org/10.1002/chem.200601792>
78. Ground and Excited States of Singlet, Cation Doublet, and Anion Doublet States of o-Benzoquinone: A Theoretical Study,  
Y. Honda, M. Hada, M. Ehara, H. Nakatsuji, *J. Phys. Chem. A*, **111**, 2634-2639 (2007).  
**DOI:** [10.1021/jp0686487](https://doi.org/10.1021/jp0686487)
79. Applicability of the lowest-order two-electron Breit-Pauli relativistic correction in many-electron heavy and super-heavy elements,  
J. Seino, M. Hada, *Chem. Phys. Letters*, **442**, 134-139 (2007).  
**DOI:** <https://doi.org/10.1016/j.cplett.2007.05.044>
80. Excitation and circular dichroism spectra of  $(-)$ -(3aS, 7aS)-2-chalcogena-trans-hydridans(Ch = S, Se, Te): SAC and SAC-CI calculations,

Y. Honda, A. Kurihara, M. Hada, H. Nakatsuji, *J. Comp. Chem.*, **29**, 612-621 (2008).

**DOI:** <https://doi.org/10.1002/jcc.20818>

81. Effect of Tridentate Ligand on Structure, Electronic Structure, and Reactivity of Copper(I) Nitrite Complex: Role of Conserved Three-Histidines Ligand Environment of Type-2 Copper Site in Copper Containing Nitrite Reductase,  
M. Kujime, C. Izumi, M. Tomura, M. Hada, H. Fujii, *J.A.C.S.*, **130**(19) 6088-6098 (2008).  
**DOI:** 10.1021/ja075575b
82. Evaluation of Electron Population Terms for  $\langle rSe-3 \rangle 4p$ ,  $\langle rS-3 \rangle 3p$ , and  $\langle rO-3 \rangle 2p$ : How Do HOMO and LUMO Shrink or Expand Depending on Nuclear Charges?,  
W. Nakanishi, S. Hayashi, K. Narahara, D. Yamaki, M. Hada, *Chemistry A European J.*, **14**, 7278-7284 (2008).  
**DOI:** <https://doi.org/10.1002/chem.200800264>
83. An ab initio study based on a finite nucleus model for isotope fractionation in the U(III)-U(IV) exchange reaction system,  
M. Abe, T. Suzuki, Y. Fujii, M. Hada, *J. Chem. Phys.*, **128**(14), 1443096(2008).  
**DOI:** <https://doi.org/10.1063/1.2898541>
84. Relativistic quantum-chemical calculations of magnetizabilities of noble gas atoms using the Douglas-Kroll-Hess method,  
T. Yoshizawa M. Hada, *Chem. Phys. Letters*, **458**, 223-226 (2008).  
**DOI:** <https://doi.org/10.1016/j.cplett.2008.04.068>
85. Contributions from atomic p(Se), d(Se), and f(Se) Orbitals to Absolute Paramagnetic Shielding Tensors in Neutral and Charged SeH<sub>n</sub> and Some Oxides, Together with the Effect of Methyl and Halogen Substitutions on sigma-p(Se),  
W. Nakanishi, S. Hayashi, K. Narahara, M. Hada, *Chemistry A European J.*, **14**, 9647-9655 (2008).  
**DOI:** <https://doi.org/10.1002/chem.200500927>
86. Examination of accuracy of electron-electron Coulomb interactions in two-component relativistic methods,  
J. Seino, M. Hada, *Chem. Phys. Letters*, **461**, 327-331 (2008).  
**DOI:** <https://doi.org/10.1016/j.cplett.2008.07.009>
87. An ab initio molecular orbital study of the nuclear volume effects in uranium isotope fractionations,  
M. Abe, T. Suzuki, Y. Fujii, M. Hada, K. Hirao, *J. Chem. Phys.*, **129**(16), 1643091 - 1643097 (2008).  
**DOI:** 10.1063/1.2992616

88. Natural Orbital Analysis of Difference Density Matrix of Cyanide Fe(III) Porphyrins,  
D. Yamaki, M. Suzuki, M. Hada, *AIP Conf. Proc.*, **1046**, 68-71 (2008).  
**DOI:** <https://doi.org/10.1063/1.2997318>
89. Relativistic and Electron-Correlation Effects on Magnetizabilities Investigated by the Douglas-Kroll-Hess Method and the Second-Order Moller-Plesset Perturbation Theory,  
T. Yoshizawa, M. Hada, *J. Comp. Chem.*, **30**(15), 2550-2566 (2009).  
**DOI:** <https://doi.org/10.1002/jcc.21261>
90. Critical Role of External Axial Ligands in Chirality Amplification of trans-Cyclo- hexane-1,2-diamine in Salen Complexes,  
T. Kurahashi, M. Hada, H. Fujii, *J. Am. Chem. Soc.*, **131**(34), 12394-12405 (2009).  
**DOI:** [10.1021/ja904635n](https://doi.org/10.1021/ja904635n)
91. Dilithioplumbole: A Lead-Bearing Aromatic Cyclopentadienyl Analog,  
M. Saito, M. Sakaguchi, T. Tajima, K. Ishimura, S. Nagase, M. Hada, *Science*, **328**, 339-342 (2010).  
**DOI:** [10.1126/science.1183648](https://doi.org/10.1126/science.1183648)
92. Calculations and Electronic Analyses of  $^{55}\text{Mn}$  and  $^{13}\text{C}$  Nuclear Magnetic Shielding Constants for  $\text{Mn}(\text{CO})5\text{X}$  ( $\text{X} = \text{H, F, Cl, Br, I, and CH}_3$ ) and  $\text{M}(\text{CO})(\text{NH}_3)_3$  ( $\text{M} = \text{Cr}^{2+}, \text{Fe}^{2+}, \text{Cu}^+, \text{and Zn}^{2+}$ ),  
H. Tanimura, A. Kitahori, C. Kuzuoka, Y. Honda, M. Hada, *Bull. Chem. Soc. Japan*, **83**, 514-519 (2010).  
**DOI:** <https://doi.org/10.1246/bcsj.20090344>
93. Erratum:An ab initio molecular orbital study of the nuclear volume effects in uranium isotope fractionations,  
M. Abe, T. Suzuki, Y. Fujii, M. Hada, K. Hirao, *J. Chem. Phys.*, **132**, 119902 (2010).  
**DOI:** <https://doi.org/10.1063/1.3357985>
94. A Hybrid-Type Data Base: Quantum Chemistry Literature Data Base II- New Concept and New Methodology -,  
K. Takano, N. Koga, T. Matsushita, K. Hashimoto, H. Hosoya, H. Matsuzawa, U. Nagashima, T. Nishikawa, H. Wasada, S. Yamabe, M. Tachikawa, M. Hada, *Bull. Chem. Soc. Japan*, **83**(5), 514-519 (2010).  
**DOI:** <https://doi.org/10.1246/bcsj.20100042>
95. Expectation values in two-component relativistic theories,  
J. Seino, W. Uesugi, M. Hada, *J. Chem. Phys.*, **132**(16), 164108(1-9) (2010).  
**DOI:** <https://doi.org/10.1063/1.3397070>
96. Magnetic shielding constants calculated by the infinite-order Douglas-Kroll-Hess method with electron-electron relativistic corrections,

J. Seino M. Hada, *J. Chem. Phys.*, **132**(17), 174105(1-8) (2010).

**DOI:** <https://doi.org/10.1063/1.3413529>

97. Excitation and Circular Dichroism Spectra of (+)-(S,S)-bis(2-methylbutyl) chalcogenides,

Y. Honda, A. Kurihara, Y. Kenmochi, M. Hada, *Molecules*, **15**, 2357-2373 (2010).

**DOI:** 103390/molecules15042357

98. Relativistic calculations of ground and excited states of LiYb molecule for ultracold photo association spectroscopy studies,

G. Gopakumar, M. Abe, B. P. Das, M. Hada, K. Hirao, *J. Chem. Phys.*, **133**(12), 124317 (2010).

99. Unique properties and reactivity of high-valent manganese-oxo versus manganese-hydoro in the salen platform"

T. Kurahashi, A. Kikuchi, Y. Shiro, M. Hada, H. Fujii, *Inorg. Chem.*, **49**(14), 6664-6672 (2010).

100. Ligand effect on uranium isotope fractionations caused by nuclear volume effects: an ab initio relativistic molecular orbital study,

M. Abe, T. Suzuki, Y. Fujii, M. Hada, K. Hirao, *J. Chem. Phys.*, **133**, 044309 (2010).

**DOI:** <https://doi.org/10.1063/1.3463797>

101. Ab initio study on vibrational dipole moments of XH<sup>+</sup> molecular ions: X = <sup>24</sup>Mg, <sup>40</sup>Ca, <sup>64</sup>Zn, <sup>88</sup>Sr, <sup>114</sup>Cd, <sup>138</sup>Ba, <sup>174</sup>Yb, and <sup>202</sup>Hg,

M. Abe, M. Kajita, M. Hada, Y. Moriwaki, *J. Phys. B: At. Mol. Opt. Phys.*, **43**, 245102-245112 (2010).

**DOI:** 10.1016/j.cplett.2011.11.048

102. Nuclear Magnetic Shielding and Aromaticity of [18]Annulene and its Quasi- Möbius-Type Analogues,

H. Tanimura, Y. Honda, K. Sugiura, M Hada, *Bull. Chem. Soc. Japan*, **84**(8), 845-854 (2011).

**DOI:** 10.1246/bcsj.20100257

103. An Equation-of-Motion Coupled-Cluster Method using Generalized Spin-Orbital Functions Including Spin-Orbit Interactions,

T. Matsuoka, S. Someno, M Hada, *J. Comp. Chem. Japan*, **10** (1), 11-17 (2011).

**DOI:** 10.2477/jccj.H2219

104. Estimated accuracies of pure XH<sup>+</sup> ( X :even isotopes of group II atoms) vibrational transition frequencies: Toward the test of the variance in mp/me,

M. Kajita, M. Abe, M. Hada, Y. Moriwaki, *J. Phys. B: At. Mol. Opt. Phys.*, **44**(2), 025402-025408 (2011).

**DOI:** 10.1088/0953-4075/44/2/025402

105. Relativistic Effect on  $^{77}\text{Se}$  NMR Chemical Shifts of Various Selenium Species in the Framework of Zeroth-Order Regular Approximation,  
W. Nakanishi, S. Hayashi, Y. Katsura, M. Hada, *J. Phys. Chem. A*, **115**(31), 8721-8730 (2011).  
**DOI:** 10.1021/jp202278f
106. Elimination of the Stark shift from the vibrational transition frequency of optically trapped  $^{174}\text{Yb}^6\text{Li}$  molecules,  
M. Kajita, G. Gopakumar, M. Abe, M. Hada, *Phys. Rev A*, **84**(2), 022507-022512 (2011).  
**DOI:** 10.1103/PhysRevA.84.022507
107. Ab initio study of permanent electric dipole moment and radiative lifetimes of alkali-earth-Li molecules,  
G. Gopakumar, M. Abe, M. Kajita, M. Hada, *Physical Review A*, **84**(6), 062514-062520 (2011).  
**DOI:** 10.1103/PhysRevA.84.062514
108. Magnetic-field effects in transitions of X Li molecules (X: even isotopes of group II atoms),  
G. Gopakumar, M. Abe, M. Hada, M. Kajita, *Phys. Rev A*, **84**(4), 045401 (2011).  
**DOI:** 10.1103/PhysRevA.84.045401
109. Ab initio study on potential energy curves of electronic ground and excited states of  $^{40}\text{CaH}^+$  molecule,  
M. Abe, Y. Moriwaki, M. Hada, M. Kajita, *Chem. Phys. Letters*, **521**, 31-35 (2011).  
**DOI:** <https://doi.org/10.1016/j.cplett.2011.11.048>
110. Effect of the Axial Ligand on the Reactivity of the Oxoiron(IV) Porphyrin  $\pi$ -Cation Radical Complex:  
Higher Stabilization of the Product State Relative to the Reactant State,  
A. Takahashi, D. Yamaki, K. Ikemuma, T. Kurahashi, T. Ogura, M. Hada, H. Fujii, *Inorg. Chem*, **51**(13), 7296-7305 (2012).  
**DOI:** [org/doi/10.1021/ic3006597](http://org/doi/10.1021/ic3006597)
111. Accuracy estimations of overtone vibrational transition frequencies of optically trapped  $^{174}\text{Yb}^6\text{Li}$  molecules,  
M. Kajita, G. Gopakumar, M. Abe, M. Hada, *Phys. Rev. A*, **85**(6), 062519 (2012).  
**DOI:** 10.1103/PhysRevA.85.062519
112. Nuclear Magnetic Shielding and Aromaticity of [18]Annulene and Its Quasi-Möbius-Type Analogues,  
H. Tanimura, Y. Honda, K. Sugiura, M. Hada, *Bull. Chem. Soc. Jpn, Additions and Corrections*, **84**(11), 1244-1244 (2012).  
**DOI:** 10.1246/bcsj.20120271

113. The Douglas-Kroll-Hess method based on vector-potential-including Foldy- Wouthuysen transformation:  
Application to NMR shielding tensor,  
T. Yoshizawa, M. Hada, *Chem. Phys. Letters*, **580**, 145-151 (2013).  
**DOI:** <https://doi.org/10.1016/j.cplett.2013.06.036>
114. Sensitivity of vibrational spectroscopy of optically trapped SrLi and CaLi molecules to variations in  $m_p/m_e$ ,  
M. Kajita, G. Gopakumar, M. Abe, M. Hada, *J. Phys. B: At. Mol. Opt. Phys.*, **46**, 025001-025005 (2013).  
**DOI:** <https://doi.org/10.1088/0953-4075/46/2/025001>
115. Oxygen-Atom Transfer from Lodosylarene Adducts of a Manganese(IV) Salen Complex: Effect of Arenes and Anions on I(III) of the Coordinated Iodosylarene,  
C. Wang, T. Kurahashi, K. Inomata, M. Hada, H. Fujii, *Inorg. Chem.*, **52**(16), 9557-9566 (2013).  
**DOI:** <http://dx.doi.org/10.1021/ic401270j>
116. Synthesis, Structure, and Reactivity of Lewis-Base-Stabilized Plumbacyclopenta- dienylidenes,  
M. Saito, T. Akiba, M. Kaneko, T. Kawamura, M. Abe, M. Hada, M. Minoura, *Chemistry A European Journal*, **19**, 16946 (2013).  
**DOI:** [10.1002/chem.201303672](https://doi.org/10.1002/chem.201303672)
117. Ab initio study of ground and excited states of  ${}^6\text{Li}{}^{40}\text{Ca}$  and  ${}^6\text{Li}{}^{88}\text{Sr}$  molecules,  
G. Gopakumar, M. Abe, M. Hada, M. Kajita, *J. Chem. Phys.*, **138**, 194307 (2013).  
**DOI:** [10.1063/1.4804622](https://doi.org/10.1063/1.4804622)
118. Theoretical Study of Isotope Enrichment Caused by Nuclear Volume Effect,  
M. Abe, T. Suzuki, Y. Fujii, M. Hada, K. Hirao, *J. Comp. Chem. Jpn.*, **13**, 92-104 (2014).  
**DOI:** [10.2477/jccj.2013-0015](https://doi.org/10.2477/jccj.2013-0015)
119. Di- $\mu$ -oxo Dimetal Core of MnIV and TiIV as a Linker Between Two Chiral Salen Complexes Leading to the Stereoselective Formation of Different M- and P- Helical Structures,  
T. Kurahashi, M. Hada, and H. Fujii, *Inorg. Chem.*, **53**, 1070-1079 (2014).  
**DOI:** [10.1021/ic402572h](https://doi.org/10.1021/ic402572h)
120. Quantum-Chemical Analyses of Aromaticity, UV Spectra and NMR Chemical Shifts in Plumbacyclopentadienylidenes Stabilized by Lewis Bases,  
T. Kawamura, M. Abe, M. Saito, M. Hada, *J. Comp. Chem.*, **35**(11), 847-853 (2014).  
**DOI:** [10.1002/jcc.23556](https://doi.org/10.1002/jcc.23556)
121. Characterizing the variation in the proton-to-electron mass ratio via precise measurement of molecular vibrational transition frequencies,

- M. Kajita, G. Gopakumar, M. Abe, M. Hada, *J. Mol. Spectroscopy*, **300**, 99-107 (2014).  
<https://doi.org/10.1016/j.jms.2014.03.009>
122. Test of  $m_p/m_e$  changes using vibrational transitions in N2+,  
M. Kajita, G. Gopakumar, M. Abe, M. Hada, M. Keller, *Phys. Rev. A*, **89**(3), 032509 (1-6) (2014).  
**DOI:** 10.1103/PhysRevA.89.032509
123. Dipole polarizability of alkali-metal (Na, K, Rb)-alkaline-earth-metal (Ca, Sr) polar molecules: Prospects for alignment,  
G. Gopakumar, M. Abe, M. Hada, M. Kajita, *J. Chem. Phys.*, **140**, 224303 (2014).  
**DOI:** <http://dx.doi.org/10.1063/1.4881396>
124. Diagonal Born-Oppenheimer Correction Based on Spin-Free Relativistic Hamiltonians,  
Y. Imafuku, M. Abe, M. W. Schmidt, M. Hada, *J. Comp. Chem. Jpn.*, **13**(4), 229-232 (2014).  
**DOI:** <http://dx.doi.org/10.2477/jccj.2014-0007>
125. Application of a Relativistic Coupled-Cluster Theory to the Effective Electric Field in YbF,  
M. Abe, G. Gopakumar, M. Hada, B. P. Das, H. Tatewaki, D. Mukherjee, *Phys. Rev. A*, **90**, 022501-022504 (2014)  
**DOI:** 10.1103/PhysRevA.90.022501
126. Ab Initio Study of Nuclear Volume Effects for Isotope Fractionations Using Two-Component Relativistic Methods,  
K. Nemoto, M. Abe, J. Seino, M. Hada, *J. Compt. Chem.*, **36**(11), 816-820 (2015).  
**DOI:** <https://doi.org/10.1002/jcc.23858>
127. Gauge-origin dependence of NMR shielding constants in the Douglas-Kroll-Hess method,  
T. Yoshizawa, M. Hada, *Chemical Physics Letters*, **618**, 132-141 (2015).  
**DOI:** <https://doi.org/10.1016/j.cplett.2014.10.066>
128. Theoretical study of the infrared frequencies of crystalline methyl acetate under interstellar medium condition,  
Radhika Narayanan, K. Inomata, G. Gopakumar, B. Sivaraman, Y. Zempo, and Masahiko Hada, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, **153**, 415-421 (2016).  
**DOI:** 10.1016/j.saa.2015.08.049
129. The functional role of the structure of the dioxo-isobacteriochlorin in the catalytic site of cytochrome cd1 for the reduction of nitrite,  
H. Fujii, D. Yamaki, T. Ogurand, M. Hada, *Chem. Science*, **7**, 2896-2906 (2016).  
**DOI:** 10.1039/c5sc04825g

130. The Origin of Relative Stability of Di- $\mu$ -oxo M-M Chiral Salen Complexes (M-M = Ti (IV)-Ti(IV), V(IV)-V(IV), Cr(IV)-Cr(IV) and Mn(IV)-Mn(IV)) : A Quantum-Chemical Analysis,  
Radhika Narayanan, A. Velloth, T. Kurahashi, H. Fujii, M. Hada, *Bull. Chem. Soc. Jpn.*, **89**, 447-454 (2016).  
**DOI:** 10.1246/bcsj.20150393
131. Relativistic coupled-cluster calculation of the electron-nucleus scalar-pseudoscalar interaction constant Ws in YbF,  
A. Sunaga, M. Abe, M. Hada, B. P. Das, *Phys. Rev. A*, **93**, 042507 (2016).  
**DOI:** 10.1103/PhysRevA.93.042507
132. Design of spin-forbidden transitions for polypyridyl metal complexes by time-dependent density functional theory including spin-orbit interaction,  
S. Kanno, Y. Imamura, M. Hada, *Phys. Chem. Chem. Phys.*, **18**, 14466-14478, (2016).  
**DOI:** 10.1039/C6CP01461E
133. Correlating Magnetic Exchange in Dinuclear Bis(phenolate)-Bridged Complexes: A Computational Perspective,  
Velloth Archana, Y. Imamura, H. Sakiyama and M. Hada, **B9**, 657-665 (2016).  
**DOI:** 10.1246/bcsj.20160077
134. N3 系色素の近赤外線光吸収の理論的設計:スピン禁制励起,  
S.kanno, Y.imamura, M.hada, *J. Comput. Chem. Jpn.*, **15** (3), 77-78 (2016).  
**DOI:** <https://doi.org/10.2477/jccj.2016-0031>
135. Synthesis and Reactivity of a Ruthenocene-type Complex Bearing an Aromatic  $\pi$ -Ligand with the Heaviest Group 14 Element,  
M. Nakada, T. Kuwabara, S. Furukawa, M. Hada, M. Minoura, M. Saito, *Chemical Science*, **8**, 2092-2097 (2017).  
**DOI:** 10.1039/C6SC04843A
136. Anisotropic Crystals Based on Main-group Coordination Polymer with Alignment of Rigid  $\pi$ -Frameworks,  
M. Saito, T. Akiba, S. Furukawa, M. Minoura, M. Hada, H. Y. Yoshikawa, *Organometallics*, **36** (14), 2487-2490 (2017).  
**DOI:** 10.1021/acs.organomet.7b00217
137. Analysis of large effective electric fields of weakly polar molecules for electron electric-dipole-moment searches  
A. Sunaga, M. Abe, M. Hada, B. P. Das, *Phys. Rev. A*, **95**, 012502 (2017).

**DOI:** 10.1103/PhysRevA.95.012502

138. Quantum Chemical Study on Endohedral Heteronuclear Dimetallofullerene M1M2@Ih-C80 Toward Molecular Design,

A. Velloth, Y. Imamura, T. Kodama, M. Hada, *J. Phys. Chem. C*, **121** (49), 27700-27708 (2017).

**DOI:** 10.1021/acs.jpcc.7b08302

139. Automatic High-Throughput Screening Scheme for Organic Photovoltaics: Estimating the Orbital Energies of Polymers from Oligomers and Evaluating the Photovoltaic Characteristics,

Y. Imamura, M. Tashiro, M. Katouda, M. Hada, *J. Phys. Chem. C*, **121** (51), 28275-28286 (2017).

**DOI:** 10.1021/acs.jpcc.7b08446

140. Theoretical Insights into the Electronic Structures and Stability of Dimetallo- fullerenes M2@Ih-C80,

A. Velloth, Y. Imamura, T. Kodama, M. Hada, *J. Phys. Chem. C*, **121** (33), 18169-18177 (2017).

**DOI:** 10.1021/acs.jpcc.7b03533

141. Rotational Energy Barriers and Relaxation Times of the Organic Cation in Cubic Methylammonium Lead/Tin Halide Perovskites from First Principles,

S. Kanno, Y. Imamura, A. Saeki, M. Hada, *J. Phys. Chem. C*, **121**, 14051-14059 (2017).

**DOI:** 10.1021/acs.jpcc.7b04589

142. Quantum Chemical Studies on Electron-Accepting Overcrowded Ethylene with a Polarizable Skeleton,

T. Tada, T. Fukushima, M. Hada, Y. Majjima, *J. Phys. Chem. A*, **121**(40), 7797-7806 (2017).

**DOI:** 10.1021/acs.jpca.7b09172

143. 4成分相対論における超微細結合定数の定式化に関する考察,

A. Sunaga, M. Abe, M. masahiko, *J. Comput. Chem. Jpn.*, **16**(4), 81-82 (2017).

**DOI:** <https://doi.org/10.2477/jccj.2017-0034>

144. 閉殻重原子系における外部静磁場によって誘起される電子スピン密度の解析,

Y. Miyamoto, Y.koyama, M.hada, *J. Comput. Chem. Jpn.*, **16**(4), 91-92 (2017).

**DOI:** <https://doi.org/10.2477/jccj.2017-0031>

145. Calculations of nuclear magnetic shielding constants based on the exact two-component relativistic method,

T. Yoshizawa, M. Hada, *J. Chem. Phys.*, **147**, 15104 (2017).

**DOI:** <https://doi.org/10.1063/1.5001256>

Selected as AIP Editors' Choice

146. Theoretical Study on Rotational Controllability of Organic Cations in Organic-Inorganic Hybrid Perovskites: Hydrogen Bonds and Halogen Substitution,  
S. Kanno, Y. Imamura, M. Hada, *J. Phys. Chem. C*, **121**(47), 26188-26195 (2017).  
**DOI:** 10.1021/acs.jpcc.7b07721

147. Vanadium NMR Chemical Shifts of (Imido)vanadium(V) Dichloride Complexes with Imidazolin-2-iminato and Imidazolidin-2-iminato Ligands: Cooperation with Quantum-Chemical Calculations and Multiple Linear Regression Analyses,  
J. Yi, W. Yang, W. Sun, K. Nomura, M. Hada, *J. Phys. Chem. A*, **121**(47), 9099-9105 (2017).  
**DOI:** 10.1021/acs.jpca.7b08328

148. Anomalous Dielectric Behavior of a Pb/Sn Perovskite: Effect of Trapped Charges on Complex Photoconductivity,  
K. Yamada, R. Nishikubo, H. Oga, Y. Ogomi, S. Hayase, S. Kanno, Y. Imamura, M. Hada, A. Saeki, *ACS Photonics*, **5**(8), 3189-3197 (2018).  
**DOI:** 10.1021/acsphotonics.8b00422

149. Theoretical study on the size-dependence of ground-state proton transfer in phenol-ammonia cluster,  
T. Shimizu, K. Hashimoto, M. Hada, M. Miyazaki, M. Fuji, *Phys. Chem. Chem. Phys.*, **20**(5), 3265-3276 (2018).  
**DOI:** 10.1039/C7CP05247B

150. First-Principles Calculations of the Rotational Motion and Hydrogen Bond Capability of Large Organic Cations in Hybrid Perovskites,  
S. Kanno, Y. Imamura, M. Hada, *J. Phys. Chem. C*, **122**(28), 15966-15972 (2018).  
**DOI:** 10.1021/acs.jpcc.8b05570

151. Extrapolation of Polymer Gap by Combining Cluster and Periodic Boundary Condition Calculations with Hückel Theory,  
Yutaka Imamura, Motomichi Tashiro; Michio Katouda; Masahiko Hada, *Chem. Phys. Letters*, **707**, 44-48, (2018). *DOI:* 10.1016/j.cplett.2018.07.023

152. Enhancement factors of parity- and time-reversal-violating effects for monofluorides,  
A. Sunaga, V. S. Prasanna, M. Abe, M. Hada, and B. P. Das, *Phys. Rev. A*, **98**, 042511(1-6), (2018).  
**DOI:** 10.1103/PhysRevA.98.042511

153. Can large active-space CASSCF calculation make sense to the reaction analysis of iron complex? A benchmark study of methane oxidation reaction by  $\text{FeO}^+$

Naoki Nakatani and Masahiko Hada, *J. Comp. Chem.*, 40(2), 414-420 (2018), (Memorial Festschrift for Keiji Morokuma)

DOI: <https://doi.org/10.1002/jcc.25640>

154. Functionalization of Endohedral Metallofullerenes toward Improving Barrier Height for the Relaxation of Magnetization for Dy<sub>2</sub>@C<sub>80</sub>-X (X = CF<sub>3</sub>, C<sub>3</sub>N<sub>3</sub>Ph<sub>2</sub>),

A. Velloth, Y. Imamura, M. Hada, *Inorganic Chemistry*, 58, 1208-1215, (2019).

**DOI:** 10.1021/acs.inorgchem.8b02652

155. Ultracold mercury-alkali-metal molecules for electron-electric-dipole-moment searches

A. Sunaga, V. S. Prasannaa, M. Abe, M. Hada, and B. P. Das, *Phys. Rev. A* **99**(4), 040501(6pages) (2019)

**DOI:** <https://doi.org/10.1103/PhysRevA.99.040501>

156. Alternative materials for perovskite solar cells from materials informatics

Shohei Kanno, Yutaka Imamura, and Masahiko Hada, *Phys. Rev. Materials* **3**, 075403(1-8), (2019).

**DOI:** 10.1103/PhysRevMaterials.3.075403

157. Substitution Effects on Olefin Epoxidation Catalyzed by Oxoiron(IV) Porphyrin p-Cation Radical

Complexes:A DFT study,

Zhifeng Ma, Kasumi Ukaji, Naoki Nakatani, Hiroshi Fujii, and Masahiko Hada, *J. Comp. Chem.*, 40(19), 1780-1788 (2019). **DOI:** <http://dx.doi.org/10.1002/jcc.25831>

158. Factors influencing the photoelectrochemical device performance sensitized by ruthenium polypyridyl dyes

Indra Purnama, Salmahaminati, Minori Abe, Masahiko Hada, Yuji Kubo, and Jacob Yan Mulyana, *Dalton Trans.*, 48, 688-695 (2019). **DOI:** 10.1039/C8DT03502D

159. The Role of Relativistic Many-Body Theory in Electron Electric Dipole Moment Searches Using Cold Molecules

V. S. Prasannaa, A. Sunaga, M. Abe, M. Hada, N. Shitara, A. Sakurai, B. P. Das, *Atoms*, 7, 58-58(20) (2019).

**DOI:**[10.3390/atoms7020058](https://doi.org/10.3390/atoms7020058)

160. Merits of heavy-heavy diatomic molecules for electron electric dipole-moment searches,

A. Sunaga, M. Abe, M. Hada and B. P. Das, *Phys. Rev. A*, 99(6), 062506-(1-7) (2019).

**DOI:**<https://doi.org/10.1103/PhysRevA.99.062506>

161. Inverted Sandwich Rh Complex Bearing a Plumbole Ligand and its Catalytic Activity,

Masaichi Saito, Marisa Nakada, Takuya Kuwabara, Ryota Owada, Shunsuke Furukawa, Radhika Narayanan, Minori Abe, Masahiko Hada, Ken Tanaka, and Yoshihiko Yamamoto, *Organometallics*, 38, 3099-3103 (2019).  
**DOI:** 10.1021/acs.organomet.9b00339

162. Computational Study on Search for Non-Fullerene Acceptors, Examination on Interface Geometry and Investigation on Electron Transfer,  
Yutaka Imamura, Marina Saganuma, and Masahiko Hada, *J. Phys. Chem. C*, 123(29), 17678-17685 (2019).  
**DOI:**<https://doi.org/10.1021/acs.jpcc.9b02933>

163. Experimental and theoretical studies of the porphyrin ligand effect on the electronic structure and reactivity of oxoiron(iv) porphyrin  $\pi$ -cation-radical complexes  
Yuri Ishimizu, Zhifeng Ma, Masahiko Hada, Hiroshi Fujii, *J. Biological and Inorganic Chemistry*, 24, 483-494 (2019). **DOI:**<https://doi.org/10.1007/s00775-019-01664-3>

164. Molecular structure and basic spectroscopic properties of 3-selenocyanatoindole: An important reference compound in organoselenium research  
Atsuki Ikeda, Shahed Ranaa, Soichi Sato, Kazunori Hirabayashi, Masahiko Hada, Toshio Shimizu, and Ken-ichi Sugiura, *Tetrahedron*, 75, 130551(1-7), (2019). **DOI:**<https://doi.org/10.1016/j.tet.2019.130551>

165.  $^{13}\text{C}$ - and  $^{207}\text{Pb}$ -NMR Chemical Shifts of Dirhodio- and Dilithioplumbole Complexes: A Quantum Chemical Assessment  
Radhika Narayanan, Marisa Nakada, Minori Abe, Masaichi Saito, Masahiko Hada, *Inorganic Chemistry*, 58(21), 14708-14719 (2019).  
**DOI:**<https://doi.org/10.1021/acs.inorgchem.9b02367>

166. Relativistic Coupled-Cluster Study of Diatomic Metal--Alkali-metal Molecules for Electron Electric Dipole Moment Searches  
Ayaki Sunaga, Minori Abe, Srinivasa Prasanna, Takatoshi Aoki, Masahiko Hada, *Journal of Physics B: Atomic, Molecular and Optical Physics*, 53(1) 015102(20). (2019). **DOI:** 10.1088/1361-6455/ab5255.

167. Time-dependent DFT study of K-edge spectra for vanadium and titanium complexes: Effects of chloride ligands on pre-edge feature  
Yi, Jun; Nakatani, Naoki; Nomura, Kotohiro; Hada, Masahiko, *Phys. Chem. Chem. Phys.* **22**, 674-682 (2020).  
**DOI:** <https://doi.org/10.1039/C9CP05891E>

168. Effect of External Electric Fields on the Oxidation Reaction of Olefins by Fe(IV)OCl-Porphyrin Complexes  
Z. Ma, H. Fujii, N. Nakatani, M. Hada, *Bulletin of Chemical Society of Japan*, 93(2), 187-192 (2020).  
**DOI:** 10.1246/bcsj.20190293

169. Exploring the Relationship between Effective Mass, Transient Photoconductivity, and Photocatalytic Activity of  $\text{Sr}_x\text{Pb}_{1-x}\text{BiO}_2\text{Cl}$  ( $x = 0\text{--}1$ ) Oxyhalides  
Hajime Suzuki, Shohei Kanno, Masahiko Hada, Ryu Abe, and Akinori Saeki, *Chemistry of Materials*, **32**(10) 4166-4173 (2020). **DOI:** <https://doi.org/10.1021/acs.chemmater.9b05366>
170. Experimental and theoretical investigation of the role of bismuth in promoting the selective oxidation of glycerol over supported Pt-Bi catalyst under mild conditions,  
Feng, Shixiang; Yi, Jun; Miura, Hiroki; Nakatani, Naoki; Hada, Masahiko; Shishido, Tetsuya, *ACS Catalysis*, **10**(11), 6071-6083 (2020). **DOI:** <https://doi.org/10.1021/acscatal.0c00974>
171. Accurate determination of the enhancement factor X for the nuclear Schiff moment in  $^{205}\text{TlF}$  molecule based on the four-component relativistic coupled-cluster theory,  
M. Abe, T. Tsutsui, J. Ekman, M. Hada, B. P. Das, *Molecular Physics*, **118**(23), e1767814, (2020).  
**DOI:** [10.1080/00268976.2020.1767814](https://doi.org/10.1080/00268976.2020.1767814)
172. Density Functional Study of Metal-to-Ligand Charge Transfer and Hole-Hopping in Ruthenium(II) Complexes with Alkyl-Substituted Bipyridine Ligands.  
Salmahaminati, \*; Abe, Minoru; Purnama, Indra; Mulyana, Jacob; Hada, Masahiko, *ACS Omega*, **6** (1), 55–64, 2021, **DOI:** <https://doi.org/10.1021/acsomega.0c01199>
173. Transition-Metal Capping to Suppress Back-Donation to Enhance Donor Ability,  
Masaichi Saito\*, Jumpei Hamada, Shunsuke Furukawa, Masahiko Hada, Libor Dostál, and Aleš Růžička, *Organometallics*, **39**(23), 4191-4194 (2020), **DOI:** <https://doi.org/10.1021/acs.organomet.0c00534>
174. Surface-enhanced Raman scattering of  $\text{M}_2\text{-pyrazine-M}_2$  ( $\text{M} = \text{Cu, Ag, Au}$ ): Analysis by natural perturbation orbitals and density functional theory functional dependence.  
Masaya Miyamoto and Masahiko Hada, *Computational Chemistry*, **41**(17), 1628-1637 (2020)  
**DOI:** <https://doi.org/10.1002/jcc.26205>
175. Theoretical study of reaction mechanism for half-titanocene-catalyzed styrene polymerization, ethylene polymerization, and styrene-ethylene copolymerization: Roles of the neutral Ti(III) and the cationic Ti(IV) species.  
Yi, Jun; Nakatani, Naoki; Tomotsu, Norio; Nomura, Kotohiro; Hada, Masahiko, *Organometallics*, **40**(6), 643-653 (2021). **DOI:** <https://doi.org/10.1021/acs.organomet.0c00715>
176.  $^{13}\text{C}$  NMR chemical shifts in substituted benzenes: analysis using natural perturbation orbitals and substitution effects.

Masaya Miyamoto and Masahiko Hada, *Mol. Phys.*, 119(6), e1843722 (2021)

**DOI:** <https://doi.org/10.1080/00268976.2020.1843722>

177. マテリアルズ・インフォマティクスを用いたペロブスカイト太陽電池材料の探索,  
菅野翔平, 今村穣, 波田雅彦, 分離技術, 50, 1, 18-24 (2020)

178. Meso-Substitution Activates Oxoiron(IV) Porphyrin  $\pi$ -Cation Radical Complex More Than  
Pyrrole- $\beta$ -Substitution for Atom Transfer Reaction.

Mami Fukui, Kanako Ueno, Masahiko Hada, Hiroshi Fujii

*Inorg. Chem.*, 60(5), 3207-3217 (2021). **DOI:** <https://doi.org/10.1021/acs.inorgchem.0c03548>

179. IR Intensities of CO Molecules Adsorbed on Atop and Low-coordinate Sites of Pd Nanoparticles: Analysis  
Using Natural Perturbation Orbitals.

Masaya Miyamoto and Masahiko Hada, *Bull. Chem. Soc. Japan*, 94(6) 1789-1793. **DOI:** 10.1246/bcsj.20210073

180. Density Functional Study on Compounds to Accelerate Electron Capture Decay of  $^7\text{Be}$ .

Akira Yoshida<sup>†</sup>, Minori Abe, and Masahiko Hada, *J. Chem. Phys. A*, 125(29), 6356-6361 (2021).

**DOI:** <https://doi.org/10.1021/acs.jpca.1c01491>

181. Synthesis, Characterization, and Reactivity of Oxoiron(IV) Porphyrin  $\pi$ -Cation Radical Complexes bearing  
Cationic 2-N-Methylpyridinium Group,

Yuna Suzuki, Masahiko Hada, and Hiroshi Fujii, *Journal of Inorganic Biochemistry*, 223, 111542 (2021).

**DOI:** [https://doi.org/10.1016/j.jinorgbio.2021.111542\(10\)](https://doi.org/10.1016/j.jinorgbio.2021.111542(10))

182. Insights into the Electronic Structure and Mechanism of Norcarane Hydroxylation by OxoMn(V) Porphyrin  
Complexes: A Density Functional Theory Study.

Zhifeng Ma, Naoki Nakatani and Masahiko Hada, *J. Comp. Chem.*, 42(26), 1920-1928 (2021).

**DOI:** <https://doi.org/10.1002/jcc.26715>

183. Rate Limiting Step of Epoxidation Reaction of Oxoiron(IV) Porphyrin  $\pi$ -Cation Radical Complex: Electron  
Transfer Coupled Bond Formation Mechanism.

Yuri Ishimizu, Zhifeng Ma, Masahiko Hada, Hiroshi Fujii, *Inorganic Chemistry*, in press

184. Utilization of diamagnetic Zn(II) ion to boost the anisotropic nature of Ln(III) ion in heterodinuclear  
Zn(II)-Ln(III) SMMs,

Soumalya Roy, Pooja Shukla, Raman Kumar, Subash Chandra Sahoo, Tapan K. Pal, Amit Rajput<sup>e</sup>, Julia Klak,  
Masahiko Hada, Kuduva R. Vignesh, Sourav Das, *Applied Organometallic Chemistry*, in press.

**DOI:** <http://doi.org/10.1002/aoc.6914>