

## Curriculum Vitae: Suehiro Iwata

(submitted for the application of the funding to the travel to Brazil, 2019)

### 1) Education/Training

1967	Dr. of Science	Graduate School of Science, University of Tokyo
1972/2–1973/8	Post- Doctorate	With Prof. Keiji Morokuma, University of Rochester
1973/9–1975/3	Post- Doctorate	With Prof. Karl Freed, University of Chicago

### 2) Professional History

#### Career History

1967/4 – 1981/3	Research Scientist, Institute of Physical and Chemical Research
1979/4 – 1981/3	Adjunct Associate Professor, Institute of Molecular Science
1981/4 – 1986/3	Associate Professor, Keio University
1986/4 – 1993/12	Professor, Keio University
1994/1 – 2000/3	Professor, Institute of Molecular Science
1994/1 – 1994/9	Adjunct Professor, Keio University
1994/4 – 2000/3	Professor, Graduate University of Advanced Study
2000/4 – present	Emeritus Professor, Institute of Molecular Science and Graduate University of Advanced Study
2000/4 – 2001/3	Professor, Graduate School of Science, Hiroshima University
2001/4 – 2004/4	Professor, National Institute of Academic Degrees and University Evaluation
2001/4 – 2001/9	Adjunct Professor, Graduate School of Science, Hiroshima University
2002/4 – 2003/3	Adjunct Professor, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University
2004/5 – 2008/3	Specially Appointed Professor, Quantum Life Sciences and Graduate School of Science, Hiroshima University
2008/4 – 2012/3	Fellow, Toyota Physical and Chemical Research Institute
2012/4 – present	Visiting Professor, Keio University

#### Organizational positions

1994/4 – 2000/3	Director, Computer Center, Institute of Molecular Science
1981/4 – 1984/3	Editorial board, Bulletin of Chemical Society of Japan
1984/3 – 1987/3	Associate Editor, Bulletin of Chemical Society of Japan
1986 – 1993	Specialist editor, Computer Physics Communication
1994 – 1997	Editorial board, Theoretica Chimica Acta

1997 – 2007 Editorial board, Theoretical Chemistry Accounts

1999 – 2001 Editorial board, Molecular Physics

**Award**

2000/3 Japanese Chemical Society Award

**3) 10 most relevant scientific results**

Electronic origin of the dependence of hydrogen bond strengths on nearest-neighbor and next-nearestneighbor-hydrogen bonds in polyhedral water clusters,  $(\text{H}_2\text{O})_n$ ,  $n=8, 20$  and  $24$ . Suehiro Iwata, Dai Akase, Misako Aida, Sotiris Xantheas, PCCP, 18 (2016) 19746 – 19756, DOI:10.1039/c6cp02487d

Analysis of hydrogen bond energies and hydrogen bonded networks in water clusters  $(\text{H}_2\text{O})_n$ ,  $n \leq 25$ . 25. Importance of cooperation of charge-transfer and dispersion terms, Suehiro Iwata, Phys. Chem. Chem.Phys. 16 (2014).11310 – 11317, DOI:10.1039/C4CP01204F.

Ab initio molecular orbital studies on paracyclophanes and siloxane-bridged paracyclophan, Soichi Shirai, Suehiro Iwata, Yoshifumi Maegawa, Takao Tani, Shinji Inagaki, J. Phys. Chem. A, 116 (2012) 10197 – 10202, DOI:10.1021/jp306416x/

Energy analysis of weak electron-donor-acceptor complexes and water clusters with the perturbation theory based on the locally projected molecular orbitals: charge-transfer and dispersion terms, Suehiro Iwata, Physical Chemistry and Chemical Physics, 14 (2012) 7787 - 7794, DOI:10.1039/C2CP40217C.

Ab initio Studies of Aromatic Excimers with Multiconfigurational Quasi-degenerated Perturbation Theory, Soichi Shirai, Suehiro Iwata, Takao Tani, and Shinji Inagaki, J.Phys.Chem. A, 115 (2011) 7687-7699 DOI:10.1021/jp201130k

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

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

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

Accurate evaluation of Einstein's A and B coefficients of rovibrational transitions for carbon monoxide: Spectral simulation of  $D_v=2$  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

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, J. Chem. Phys. 115 (2001) 3553-3560

**4) List of financial grants**

1998–2002 “Computational Chemistry for Atmospheric Environmental Molecules”, supported by Japan Science and Technology Corporation.

**5) Research projects under way which are financed by a fellowship or scholarship**

Nothing to declare

**6) Academic Quantitative Indicators**

Books: none

Publications in peer-reviewed international journals: 231

Review Articles (Peer-reviewed): 25

Supervised and concluded Master's dissertations: more than 30

Supervised and concluded Doctoral theses: 12

ResearchGate: RG score 43.39, h-index:43, h-index(excluding self-citations):42

Google Scholar: h index:50, i10 index:185, citation:9808

**7) MyResearcherID (ISI):** [None](#)

**8) Other Information:** Nothing to declare