THE JOURNAL OF PHYSICAL CHEMISTRY A

Viewpoint

Cite This: J. Phys. Chem. A 2018, 122, 880−881

pubs.acs.org/JPCA

Keiji Morokuma

It is with great sadness that we mark the passing of Keiji Morokuma on November 27, 2017. Keiji Morokuma was a giant in the field of electronic structure theory and applications. Keiji received his Ph.D. from Kyoto University, under the direction of Kenichi Fukui in 1963. He was Research Associate (junior faculty), Kyoto University, 1962−66, and a postdoc from 1966 to 67 at Harvard University with Martin Karplus. In 1967, Morokuma joined the Chemistry Department of University of Rochester as an Assistant Professor. He rose rapidly through the ranks, becoming a Full Professor in 1971. He moved to Japan in 1976 to become Professor, and shortly later Director, of the Dept. of Theoretical Studies, Institute for Molecular Science, Okazaki, Japan. From 1978 to 93 he was also Director of the Computer Center of the Institute for Molecular Science. He returned to the US in 1993 to become Director of the Cherry L. Emerson Center for Scientific Computation and William Henry Emerson Professor of Chemistry at Emory University. Keiji became William Henry Emerson Professor Emeritus, Emory University, in 2006 and took up his final academic position as Research Leader, Fukui Institute for Fundamental Chemistry, Kyoto University.

Keiji authored or coauthored more than 900 papers, many review articles and several books. He received numerous awards, including The Chemical Society Award, The Chemical Society of Japan (1992), the Schrödinger Medal, The World Association of Theoretical Organic Chemists (1993), the Bourke Lectureship, Faraday Division, Royal Society of Chemistry, U.K. (1990), the Fukui Medal, Asian Pacific Association of Theoretical & Computational Chemists (2005), the Imperial Prize and the Japan Academy Prize, the Japan Academy (2008), Person of Cultural Merit, Japan (2009), and The Emerson Center Lectureship Award, USA (2014).

Keiji served the community as director of scientific centers, as president of the International Academy of Quantum Molecular Sciences (from 2000 to 2006), of which he was a member since 1985, and in many editorial roles on the leading journals of the field.

Keiji made numerous seminal contributions to Theoretical and Computational Chemistry (see Table 1). The **ONIOM method** and applications to large, complex molecular systems was an inspired and now widely used hybrid approach. In this method, a molecular system is divided into several regions where an accurate QM method is used for the most important region and less time-consuming methods, e.g., molecular mechanics or low-level semiempirical methods are used for less important regions. Keiji used this method to study complex problems, such as

Table 1. Selected *J. Phys. Chem.* Publications of Keiji Morokuma

title	author(s)	citation
ONIOM: A Multilayered Integrated Mo+ Mm Method for Geometry Optimizations and Single Point Energy Predictions. A Test for Diels−Alder Reactions and $Pt(P(t\text{-}Bu)_3)_2 + H_2$ Oxidative Addition	M. Svensson, S. Humbel, R. D. J. Froese, T. Matsubara, S. Sieber, K. Morokuma	*J. Phys. Chem.* **1996**, *100*, 19357. DOI: 10.1021/jp962071j
The C_{60} Formation Puzzle Solved: QM/MD Simulations Reveal the Shrinking Hot Giant Road of the Dynamic Fullerene Self-Assembly Mechanism	S. Irle, G. Zheng, Z. Wang, K. Morokuma	*J. Phys. Chem. B* **2006**, *110*, 14531. DOI: 10.1021/jp061173z
Coexistence of neutral and ion-pair clusters of hydrated sulfuric acid H_2SO_4 $(H_2O)_n$ (n = 1−5) A molecular orbital study	S. Re, Y. Osamura, K. Morokuma	*J. Phys. Chem. A* **1999**, *103*, 3535. DOI: 10.1021/jp984759x
Application of the New Integrated MO + MM (IMOMM) Method to the Organometallic Reaction $Pt(PR_3)_2 + H_2$ (R = H, Me, *t*-Bu, and Ph)	T. Matsubara, F. Maseras, N. Koga, K. Morokuma	*J. Phys. Chem.* **1996**, *100*, 2573. DOI: 10.1021/jp951762x
Theoretical Study of Potential Energy Surface and Thermal Rate Constants for the $C_6H_5 + H_2$ and $C_6H_6 + H$ Reactions	A. M. Mebel, M. C. Lin, T. Yu, K. Morokuma	*J. Phys. Chem. A* **1997**, *101*, 3189. DOI: 10.1021/jp9702356
Ab Initio Potential Energy Surface and Electron Correlation Effect in CH Activation of Methane by Coordinatively Unsaturated Chlorodiphosphinerhodium(I)	N. Koga, K. Morokuma	*J. Phys. Chem.* **1990**, *94*, 5454. DOI: 10.1021/j100377a007
Structure, Stability, and Bonding of Transition-Metal−Boryl Complexes. A Molecular Orbital Study	D. G. Musaev, K. Morokuma	*J. Phys. Chem.* **1996**, *100*, 6509−6517. DOI: 10.1021/jp953143u
Calculation of Nuclear Quadrupole Parameters in Imidazole Derivatives and Extrapolation to Coenzyme B12. A Theoretical Study	M. Torrent, D. G. Musaev, K. Morokuma, S. C. Ke, K. Warncke	*J. Phys. Chem. B* **1999**, *103*, 8618. DOI: 10.1021/jp991612c
The role of the Central Atom in Structure and Reactivity of Polyoxometalates with Adjacent D-Metal Sites. Computational and Experimental Study of γ-$[(X^{n+}O_4)Ru_2(OH)_2W_{10}O_{30}]^{(8-n)-}$, X = Al^{III}, Si^{IV}, P^{V}, and S^{VI}	D. Quiñonero, Y. Wang, K. Morokuma, I. A. Khavrutskii, B. Botar, Y. V. Geletii, C. L. Hill, D. G. Musaev	*J. Phys. Chem. B* **2006**, *110*, 170. DOI: 10.1021/jp054728j
Is Protein Surrounding the Active-Site Critical for Hydrogen Peroxide Reduction by Selenoprotein Glutatione Peroxidase (GPx)? An ONIOM Study	R. Prabhakar, T. Vreven, M. J. Frisch, K. Morokuma, D. G. Musaev	*J. Phys. Chem. B* **2006**, *110*, 13608. DOI: 10.1021/jp0619181
Photodissociation Dynamics of Formaldehyde Initiated at the T1/S0 Minimum Energy Crossing Configurations	B. C. Shepler, E. Epifanovsky, P. Zhang, J. M. Bowman, A. I. Krylov, K. Morokuma	*J. Phys. Chem. A* **2008**, *112*, 13267. DOI: 10.1021/jp808410p
Systematic Exploration of Minimum Energy Conical Intersection Structures near the Franck−Condon Region	S. Maeda, Y. Harabuchi, T. Taketsugu, K. Morokuma	*J. Phys. Chem. A* **2014**, *118*, 12050. DOI: 10.1021/jp507698m

Published: February 1, 2018

DOI: 10.1021/acs.jpca.8b00070
J. Phys. Chem. A 2018, 122, 880−881

design of homogeneous and bioinspired catalysts (for example, Wilkinson catalysis, olefin polymerization and dinitrogen activation), prediction of chemical properties of large molecules, understanding of highly selective organic transformations, and the study of relationships between the structure and reactivity of metalloenzymes, to name a few.

Keiji also used a combined electronic structure and molecular dynamics theories to study **the mechanism of formation of fullerenes**. He proposed the "hot shrinking giant fullerene" mechanism in which self-assembly of small carbon species produces thermally excited giant fullerenes, which subsequently in the annealing process eject C_2 and other small species to reach C_{60} and other fullerenes.

Keiji's great interest in chemical reactions led him to the development of energy gradient and artificial force techniques to automatically determine reaction pathways and **mechanisms of chemical reactions**. One prominent example was the discovery of roaming in electronically excited states, and in particular the roaming pathways in the photodissocation of NO_3 to $NO + O_2$ in both the ground and first electronic states. He also used these methods to study the mechanism of complex homogeneous catalysis by transition metal complexes, for example, the hydroformylation reaction.

Keiji was pioneer in computational studies of **photochemical processes in biomolecular systems.** For example, he studied the nature of active species and mechanisms of photoconversion of reversibly photoswitchable fluorescent protein Dronpa, the green-to-red photoconversion mechanism of fluorescent protein Kaede, and the spectral tuning of visual pigment consisting of retinal Schiff base (SB) chromophore in various animals.

Keiji's **"Morokuma-Kitaura energy decomposition" method**, developed in 1976, remains an actively used approach in the analysis of molecular interactions in complexes systems.

Keiji was a loving husband of gracious and caring Eiko, father of three sons and one daughter, and grandfather of two grandchildren. He will be remembered by his many colleagues and friends for the high energy and zest that he applied to science, tennis and laughter. He was remarkably thorough in everything he did, including his power-point presentations.

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Notes

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The authors declare no competing financial interest.

DOI: 10.1021/acs.jpca.8b00070
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