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INTRODUCTION

A Festschrift in honor of Shigeru Nagase

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As numerous other world leaders in quantum and computational chemistry, Shigeru Nagase, professor at the Institute for Molecular Science or IMS in Okazaki, crosses the age of 65. This impressive wave of sexagenarians among chemical theorists is undoubtedly related to the advancements of the third-generation computers in the sixties. He was born and raised in Osaka, a town known for practical approaches of its folks. Early modern Japan revolved around three cities: the spiritual center and emperor's seat of Kyoto, the shogun's city of Edo/Tokyo, and the craft and merchant center of Osaka. People raised in Osaka are straightforward, fast-thinking, practical, tough, but warm and kind, aiming at a visible, applicable result, and frequently also heavy smokers—and he is no exception to the rules.

Shigeru received his PhD degree in 1975 (under Prof. Takayuki Fueno) from Osaka University, one of the traditional seven members of the Japanese 'Ivy League'. After three years as a postdoctoral fellow at the University of Rochester (with Prof. Keiji Morokuma) and The Ohio State University (with Prof. C. William Kern), and an intermission at the IMS in Okazaki, he became Associate Professor at Yokohama National University and Professor there in 1991. In 1995, he moved to Tokyo Metropolitan University and since 2001, he has been Professor in the Department of Theoretical and Computational Molecular Science of the IMS.

An old depiction of the present IMS area—a woodcut from 'The Fifty-Three Stations of the Tokaido' by the great Utagawa Hiroshige (1797–1858). The founder of the Tokugawa Shogunate (1603–1868), Ieyasu Tokugawa (1543–1616), was born in the Okazaki castle. The IMS campus is located to the *right* from the castle

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Shigeru has been active in several research areas like design and development of new aromatic, multiply bonded, hypervalent, polycyclic, and polyhedral compounds with heavier main group elements in the framework, including cage-like silicon and germanium clusters stabilized by transition metals. From the early days of fullerene science, he has been one of the leaders of the calculations on fullerenes, endofullerenes, nanotubes, nanographenes, peapods, nanocables, always in a close contact and co-operation with experimentalists. These days he has been interested in high-performance algorithms for MP2 and RI-MP2 calculations or in developing a projector Monte Carlo method for full-CI energies. His life-long scientific philosophy is a strong belief that the fruitful interplay between theory and experiment is mutually very important.

The future is bright for the Japanese quantum molecular science as it activities are to be supported also by the new 'K computer' (68,544 CPUs) co-ordinated by RIKEN (The Institute of Physical and Chemical Research). With such hardware background, powerful computational nanoscience of the 21-st century will flourish. In such exciting times and with a large body of disciples, collaborators, friends of Shigeru, it has been a pleasant task to organize this Festschrift.

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