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Publisher *Taylor & Francis*

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## **Molecular Simulation**

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713644482>

## **Guest Editorial: Nosé Memorial**

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**To cite this Article** Okamoto, Yuko(2007) 'Guest Editorial: Nosé Memorial', *Molecular Simulation*, 33: 1, 1 – 3

**To link to this Article:** DOI: 10.1080/08927020601105696

**URL:** <http://dx.doi.org/10.1080/08927020601105696>

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## Guest Editorial: Nosé Memorial

This issue of Molecular Simulation is dedicated to the memory of Shuichi Nosé, who passed away on August 17, 2005 at the age of 54.

The issue contains contributions from participants at the *Symposium on Progress and Future Prospects in Molecular Dynamics Simulation—In Memory of Professor Shuichi Nosé*. The Symposium was held at Keio University in Yokohama, Japan on June 6–8, 2006. The organizers were Nosé's colleagues at Keio University, his former teacher, and his former students: Hiroyuki Hyuga (Chair), Hiroshi Takano, Ayori Mitsutake (all at Department of Physics, Keio University), Kenji Yasuoka (Department of Mechanical Engineering, Keio University), Yosuke Kataoka (Department of Materials Chemistry, Hosei University), Tetsuya Morishita (Research Institute for Computational Sciences, National Institute of Advanced Industrial Science and Technology), and Hisashi Okumura (Department of Physics, Nagoya University).

Nosé was born in the city of Kyotango, Kyoto Prefecture, Japan on June 17, 1951. He graduated from Kyoto University, where he majored in chemistry. He then continued his graduate studies at the Chemistry Department, Kyoto University and studied theoretical chemistry. In 1981 he received his PhD degree under the supervision of Tsunenobu Yamamoto. Nosé then became a postdoctoral research associate at Michael L. Klein's

Laboratory in National Research Council Canada in May, 1981, where he invented the famous Nosé method for canonical-ensemble molecular dynamics simulations. In April 1984, Nosé joined as Joshi ( $\approx$  assistant professor) to the Theoretical Physics Group at the Department of Physics, Keio University, where he remained until his death. The Group was then led by Ryogo Kubo, and Nosé collaborated with Fumiko Yonezawa. He was later promoted to lecturer, associate professor, and eventually to professor there. For more details of Nosé's career, the reader is referred to an obituary by Yosuke Kataoka and Michael L. Klein in the February 2006 issue of *Physics Today*.

Nosé was a founding father of the molecular dynamics methods, that exactly reproduce the canonical ensemble including the momentum space. The development followed the two paths: from Nosé to (1) Nosé–Hoover and Nosé–Hoover chain and to (2) Nosé–Poincaré, the last of which gives a symplectic integrator. Nosé himself contributed to the first (in 1984) and the last (in 2001) in this list. His passing was indeed a great loss to the field of molecular simulation.

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Symposium on Progress and Future Prospects in Molecular Dynamics Simulation  
– In Memory of Professor Shuichi Nosé –  
Faculty of Science and Technology, Keio University, Yokohama, Japan, June 6–8, 2006



Shuichi Nosé (June 17, 1951–August 17, 2005)