744th ASRC Seminar

Date：平成31年3月8日(金)　16：00～

Location： 先端基礎研究交流棟2階
第2センター会議室

Speaker：志賀　基之
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Title：Recent Advances in Quantum Simulations of Aqueous Solutions

Abstract:

In this presentation, I will introduce some recent advances in quantum molecular dynamics simulations of aqueous solutions. One is a simulation of complex reactive processes taking place in water by locating the free energy minima and saddle points [1]. The other is a first-principles simulation that takes account of nuclear quantum effects based on imaginary-time path integral theory for a proper description of isotope effects of water [2]. I will also mention a technical advance in the QM/MM simulations using ab initio quantum chemistry to predict accurately the hydration structures of ions in water [3].

[1] M. Shiga, M. E. Tuckerman, J. Phys. Chem. Lett. 9, 6207–6214 (2018).
[2] M. Machida, K. Kato, M. Shiga, J. Chem. Phys. 148, 102324 (2018).
[3] M. Shiga, M. Masia, J. Chem. Phys. 139, 044120 (2013); 139, 144103 (2013).

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