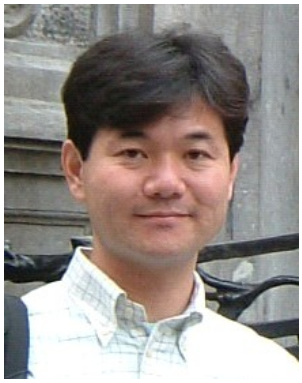
Masanori Tachikawa



Professor, Graduate School of Bionanoscience, Yokohama city University

【E-mail】 **tachi@yokohama-cu.ac.jp**

【Speciality】**Quantum Chemsitry**

【Keywords】**Multi-component molecular theory, Path Integral, Hydrogen bonding, Positronic system**

【Research Subject】

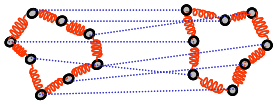
Theoretical Analysis of Supra Biomolecular Clusters Including Nuclear Quantum and Thermal fluctuations

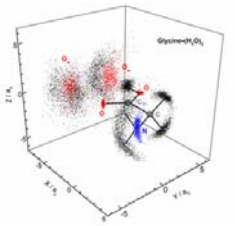
Research Group Activity

- *Ab initio* Path Integral method

Path integral and *ab initio* MO methods for nuclei and electrons to achieve *full* quantum calculations

$$Z = Tr\left(e^{-\beta\hat{H}}\right) = Tr\left(e^{-\beta\hat{H}/P}\right)^{P}$$





- Multi-component *ab initio* method

Extension of the concept of molecular orbital to nuclear motions

HF level

$$f^{e}\varphi_{i}^{e} = \varepsilon_{i}^{e}\varphi_{i}^{e}$$

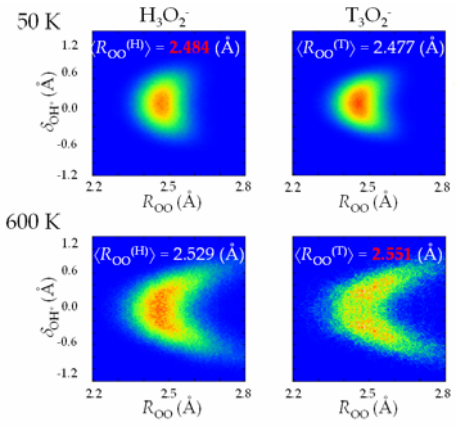
$$f^{p}\varphi_{p}^{p} = \varepsilon_{p}^{p}\varphi_{p}^{p}$$

CI level

$$\left\langle \Phi_{I}^{e} \middle| \left\langle \Phi_{J}^{p} \middle| \hat{H}_{tot} \middle| \Phi_{I'}^{e} \right\rangle \middle| \Phi_{J'}^{p} \right\rangle$$

- Low barrier hydrogen bonding

H/D isotope effects on geometry and electronic structure for LBHB systems



- Positronic compound

Theoretical study of positronic systems