Prof. Koichi Yamasahita

THE UNIVERSITY OF TOKYO DEPARTMENT OF CHEMICAL SYSTEM ENGINEERING

YAMASHITA & USHIYAMA LABORATORY

Introduction

The mission of Yamashita-Ushiyama laboratory is theoretical elucidation and control of chemical reaction dynamics. Our research interest varies from foundamental theories such as quantum chemistry and semiclassical dynamics to more application side, as computational chemistry and modeling of catalysis. Based on the methodology of the theoretical chemistiry, we are pursuing the development of the *ab initio* chemistry.

Koichi Yamashita

Koichi Yamashita's research lab is in the Department of Chemical System Engineering at the University of Tokyo.
His undergraduate and graduate degrees are from Kyoto University, where his research field was the theory of chemical reactions. He was a postdoctoral fellow with William Miller at the University of California, Berkeley, from 1982-1984. He has been a professor at the University of Tokyo since 1994. His research group varies in size typically between 7 and 15, with undergraduate and graduate students, postdoctoral fellows/junior faculty, and visiting international scholars.

Research Activities

Quantum Control of Chemical Reaction Dynamics

We study the laser control of chemical reaction dynamics in gas phase and on surfaces based on quantum chemistry and quantum wavepacket calculations. Interactions of ultra-short laser pulses with molecules, photoinduced surface reactions by femto-second lasers, laser cooling of a molecule, molecular quantum information, effects of quantum dissipation in quantum control, are current research themes. It is our dream to control molecules and chemical reactions at will.

- "Theoretical study on the structures and reactions of interstellar molecules by ab initio molecular orbital methods"
- "Molecular quantum computer and molecular quantum information theory"

Computational Reaction Chemistry on Surfaces

Many interesting phenomena of surface chemistry result from the microscopic interactions between adsorbed molecules and surfaces. In this study, we perform the first-principle calculations of the

elementary reactions of CVD processes, the photocatalitic process of TiO2, and the electron transfer reactions and molecular electronics on electrode surfaces. In addition, we challenge to construct a theoretical model of electronically excited states of surfaces.

Theoretical Design of Semiconductor Materials

With refinement of gate stack and interconnect module technology it is indispensable to develop new semiconductor materials. In order to develop new materials for high-k gate and low-k insulation membranes, we study theoretical methodology for materials design based on quantum chemistry calculations. In addition, the electron hole transfer between DNA nucleobases and optical properties of semiconductor CdSe nanocrystals are studied theoretically for new molecular devices in nano-scale electronics.

- "Metal Nanoparticle Optics by Classical Electrodynamics"
- "Theoretical study on charge transfer in native and chemically modified DNA and quantum electron transport in molecular junctions"

Molecular quantum computer and molecular quantum information theory

In physics, quantum computers and quantum information theory are investigated extensively. The focus of my research is put on the fundamental principle of molecular quantum computers, regarding molecular electronic, vibrational, and rotational degrees of freedom as qubits. In addition, I am engaged in the theoretical study on molecular entanglement, e.g., control theory and entanglement degree. My final purpose is to create a new chemistry research field (molecular quantum information theory), combining chemistry and quantum information theory. Also I am interested in finding new chemical phenomena triggered by entanglement.

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