

11th Symposium on Electronic Structure Theory

Frontiers of Theoretical Chemistry and Global Perspectives

November 14 (Fri), 2025



Veune

- Waseda University, Nishi-Waseda Campus
Building 62W, 1st Floor, Conference Rooms A & B

Organized by

- Nakai Laboratory, Department of Chemistry and Biochemistry,
School of Advanced Science and Engineering, Waseda University
(Institute for Science and Engineering Project: Social Implementation of Computational Chemistry)

Co-organized by

- Waseda Research Institute for Science and Engineering

Program

12:30 ~

Registration desk opens

13:00 ~ 13:10

Opening Remarks

13:10 ~ 13:50

Invited Lecture 1 - Toni Maier (Technische Universität Braunschweig, Germany)
"The MH24 Functional - Beyond an Exact-Exchange Journey's End"

13:50 ~ 14:30

Invited Lecture 2 - Daeheum Cho (Kyungpook National University, South Korea)
"Control of Spin-polarized Electron Transport in Molecular Junctions"

14:30 ~ 14:40

Group Photo

14:40 ~ 15:30

Poster Session & Coffee Break

15:30 ~ 16:10

Invited Lecture 3 - Patchreenart Saparpakorn (Kasetsart University, Thailand)
"Binding roles of 4-isochromanone derivatives as
potent Acetylcholinesterase inhibitors targeting Alzheimer's disease"

16:10 ~ 16:50

Invited Lecture 4 - Takeshi Sato (The University of Tokyo, Japan)
"Quantum-Classical Hybrid Simulations of Quantum Many-Body Problems:
From Chemistry to Ultrafast Intense Laser Science"

16:50 ~ 17:00

Closing Remarks

17:10 ~ 18:10

Mixer

$$\Delta E^{\text{HF}} = \frac{1}{4} \sum_{i,j} \sum_{a,b}^{\text{occ.}, \text{vir.}} \frac{|\langle ij || ab \rangle|^2}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

$$\left[\sum_{A=1}^M \sum_{B=1}^M \sum_{a=1}^M \sum_{b=1}^M \frac{Z_A Z_B}{A+B} \right] \Psi = E \Psi$$

