

# JTTCC11

(The 11th Japan-Thai workshop on Theoretical and Computational Chemistry 2026)

Date and Time:

**Saturday, April 25, 2026, 9:30 - 19:00**

Venue:

**Yokohama City University** (Kanazawa-Hakkei Campus), Yokohama, Japan.

[Oral Sessions]

**Room 141 (1F), Arts Research Building**

[Poster Session & Conference Mixer]

**Entrance Hall (1F), Science Research Building**

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## Opening Remarks

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9:30 – 9:40

**Mitsunori Ikeguchi** (Yokohama City University, Japan)

9:40 – 9:50

**Masanori Tachikawa** (Yokohama City University, Japan)

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## Oral Session 1

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Chair: **Yukiumi Kita** (Yokohama City University, Japan)

9:50 – 10:15 JTTCC11\_O1

**Daisuke Yoshida** (Tohoku University, Japan)

*Chemistry with Positrons: Insights from First-Principles Calculations into Positron-Molecule Interactions*

10:15 – 10:40 JTTCC11\_O2

**Tatsuhiro Murakami** (Tokyo Metropolitan University, Japan)

*Reaction Pathway Bifurcation in Molecular Dynamics: A Dynamical View Beyond Static Potential Energy Surfaces*

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*Coffee Break (20 min.)*  
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## Oral Session 2

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Chair: **Masanori Tachikawa** (Yokohama City University, Japan)

11:00 – 11:25 JTTCC11\_O3

**Seiji Mori** (Ibaraki University, Japan)

*Theoretical Studies on Noncovalent Interactions in Homogeneous Catalysis*

11:25 – 11:50 JTTCC11\_O4

**Jun Koseki** (AIST, Japan)

*Computational Analysis of Molecular Structure and Function*

11:50 – 12:15 JTTCC11\_O5

**David S. Rivera Rocabado** (Osaka Metropolitan University, Japan)

*Toward Interpretable Heterogeneous Catalyst Prediction and Design via AI-Driven Density of States Analysis*

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*Lunch Break (60 min.)*  
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## Oral Session 3

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Chair: **Makito Takagi** (Yokohama City University, Japan)

13:15 – 13:35 JTTCC11\_O6

**Kowit Hengphasatporn** (University of Tsukuba, Japan)

*Click, Dock, Discover: Making Computational Drug Discovery Accessible*

13:35 – 13:55 JTTCC11\_O7

**Lian Duan** (University of Tsukuba, Japan)

*A Data-Driven Reaction Path Analysis Framework for Complex Enzymatic Reactions*

13:55 – 14:20 JTTCC11\_O8

**U. Deva Priyakumar** (International Institute of Information Technology Hyderabad, India)

*Chemistry Language Models for Molecule and Material Design*

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*Coffee Break (20 min.)*  
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### Oral Session 4

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Chair: **Kenichiro Saita** (Yokohama City University, Japan)

14:40 – 15:00 JTTCC11\_O9

**Anupama Sharma** (University of Tsukuba, Japan)

*Mechanistic Insights into Carbon Nanotube Dispersion in Ionic Liquids: Role of the Cation*

15:00 – 15:25 JTTCC11\_O10

**Azusa Muraoka** (Japan Woman's University, Japan)

*NEXUS Activities at JWU for Advancing Research on High-Efficiency Photovoltaic Materials and Fostering Women Researchers*

15:25 – 15:50 JTTCC11\_O11

**Kohki Oka** (Tohoku University, Japan)

*Development of Organic Energy Materials*

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*Coffee Break (20 min.)*  
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### Oral Session 5

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Chair: **Tomomi Shimazaki** (Yokohama City University, Japan)

16:10 – 16:35 JTTCC11\_O12

**Yasuteru Shigeta** (University of Tsukuba, Japan)

*Integrated computational chemistry methods for drug discovery and functional analysis of proteins*

16:35 – 17:00 JTTCC11\_O13

**Robert Szilagyi** (University of British Columbia, Canada)

*Chromium Chemistry for Energy Storage in N–H Bonds*

17:00 – 17:25 JTTCC11\_O14

**Nawee Kungwan** (Chiang Mai University, Thailand)

*Single-benzene fluorophores: Compact Near-Infrared dye for biosensing and bioimaging*

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### Closing Remarks

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17:25 – 17:30

**Masanori Tachikawa** (Yokohama City University, Japan)

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## Poster Sessions

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17:30 – 18:15

**Poster Session 1** (Posters with odd numbers)

18:15 – 19:00

**Poster Session 2** (Posters with even numbers)

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19:00 – 21:00

**Conference Mixer**

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This workshop is organized by the Graduate School of NanoBioScience (Yokohama City University), Graduate School of Medical Life Science (Yokohama City University), Muraoka Group (Japan Women's University), and NEXUS (JST), sponsored by SPRING program (Yokohama City University) and Grant-in-Aid for Scientific Research(S) (MEXT, KAKENHI), and supported by the International Affairs Office (Yokohama City University) and Grant-in-Aid for Transformative Research Areas (A) (MEXT, KAKENHI).



## List of Posters

P1	<b>Saho Kobayashi-Kajikawa</b> (Japan Woman's University, Japan) <i>Perovskite Band Gap Prediction Using Explainable Machine Learning with ML-Generated Structural Features</i>
P2	<b>Mebuki Fujitsuka</b> (Gifu University, Japan) <i>Multi-Component Density Functional Theory Study of Deuterium Isotope Effects in Caffeine Metabolism</i>
P3	<b>Hiroaki Oheda</b> (Yokohama City University, Japan) <i>Membrane Protein and Lipid Molecule Co-folding Improves Membrane-Protein Structure Prediction Accuracy</i>
P4	<b>Nao Muramatsu</b> (Japan Woman's University, Japan) <i>First-principles study on the electronic structures of 2D and 2D/3D hybrid organic-inorganic perovskites</i>
P5	<b>Miya Matsuzaki</b> (Japan Woman's University, Japan) <i>Electronic Structure Calculations on n-type Doping of Carbon Nanotubes Using Phosphine and Amine Molecules</i>
P6	<b>Daiki Takaku</b> (Yokohama City University, Japan) <i>Mechanical stability and plasticity of protein crystals through cross-linking</i>
P7	<b>Masanari Natsume</b> (Yokohama City University, Japan) <i>Nuclear quantum effects on the free-energy landscape of the O-H<sup>+</sup>...<math>\pi</math> interaction in H<sub>3</sub>O<sup>+</sup>...acetylene complex studied by path-integral molecular dynamics simulation</i>
P8	<b>Ken Inoue</b> (Yokohama City University, Japan) <i>Synthesis and Fluorescent Properties of Natural Source Derived Carbon Quantum Dots</i>
P9	<b>Hinano Koizumi</b> (Yokohama City University, Japan) <i>Phase Space Analysis of EEG in Epilepsy Patients and Correlation with Clinical Status</i>
P10	<b>Kie Araki</b> (Japan Woman's University, Japan) <i>Molecular Dynamics Study of Ligand Recognition in the Taste Receptor T1r2a-T1r3</i>
P11	<b>Yachen Zhao</b> (Yokohama City University, Japan) <i>Composition-dependent band gaps of InGaN: Investigating lattice optimization and screened energy corrections</i>
P12	<b>Miu Ashiba</b> (Yokohama City University, Japan) <i>Theoretical Analysis of Positron Binding to Halogenated Hydrocarbons</i>
P13	<b>Ayama Tokuyasu</b> (Yokohama City University, Japan) <i>Direct physical measurement of intracellular dynamics using magnetic tweezers</i>
P14	<b>Kai Travis</b> (Yokohama City University, Japan) <i>Image-based AI toxicity prediction using human hepatocyte spheroids</i>