



AIQMD2026

Summer School

Frontiers in Ab Initio Quantum Molecular Dynamics

Jul 25 – 29, 2026

College of Chemistry and Molecular Engineering, Peking University

Organizers: Jian Liu, Eberhard K. U. Gross, Daniel Escudero

Invited Speakers

Federica Agostini
Nandini Ananth
Victor Batista
Jianshu Cao
Tucker Carrington
Michele Ceotto
Rachel Crespo Otero
Basile Curchod
Garnet Chan
Weinan E
Jiali Gao
Fabien Gatti

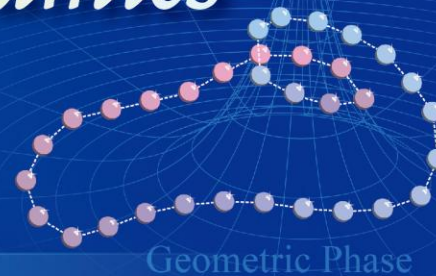
Sorbonne Univ.
Cornell Univ.
Yale Univ.
MIT
Queen's Univ.
Univ. Milan
Univ. College London
Univ. Bristol
CalTech
Peking Univ.
Univ. Minnesota
CNRS/Univ. Bourgogne Europe

Seogjoo J. Jang
Leeor Kronik
Zhenggang Lan
Shuhua Li
Xiaosong Li
Wenjian Liu
Nancy Makri
Reinhard Maurer
Akira Nakayama
Frank Neese
Francesco Paesani
Piotr Piecuch

City Univ. New York
Weizmann Institute
South China Normal Univ.
Nanjing Univ.
Univ. Washington
Shandong Univ.
UIUC
Univ. Wien
Univ. Tokyo
MPI Kohlenforschung
UCSD
Michigan State Univ.

Eli Pollak
Trond Saue
Andreas Savin
Matthias Scheffler
Dmitry Shalashilin
Zhigang Shuai
Seiichiro Ten-no
Mark Tuckerman
Christoph van Wüllen
Xin Xu
Weitao Yang
Dong Hui Zhang

Weizmann Institute
CNRS / UT3 Paul Sabatier
CNRS / Sorbonne Univ.
NOMAD Laboratory
Univ. Leeds
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Nonadiabatic Field

Sponsors:





Summer School: Frontiers in *Ab Initio* Quantum Molecular Dynamics

Xiao Lun Auditorium (C101), CCME



Monday, July 27, 2026

Yajun Liu *Session Chair*

Weitao Yang 08:30–09:10

From Functional Approximations to Excited State Theory and Computation in DFT

Jiali Gao 09:10–09:50

The One-Determines-All (ODA) Principle of MSDFT and the Design of Approximate Matrix Functionals

Run Long *Session Chair*

Leeor Kronik 10:20–11:00

Advances in Optical Spectroscopy from Density Functional Theory

Zhenggang Lan 11:00–11:40

Ab Initio Simulation of Ultrafast Spectroscopy and Nonadiabatic Dynamics in Polyatomic Molecules

Hands-on Activities 11:40–12:10

Andrey Vassenko *Session Chair*

Piotr Piecuch 14:00–14:40

H₃⁺ Formation from Methyl Halogens and Pseudohalogens: Experiment, Theory, and Governing Factors

Federica Agostini 14:40–15:20

Theory and Simulations of Ultrafast Processes in Molecules

Xuefei Xu *Session Chair*

Seogjoo J. Jang 15:50–16:30

New Theoretical Advances Towards First Principles Calculation of Fermi's Golden Rule Rates for Nonadiabatic Transitions

Akira Nakayama 16:30–17:10

Molecular Insight into the Adsorption and Conversion at the Liquid/Solid-Oxide Interface

Hands-on Activities 17:10–17:40



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Tuesday, July 28, 2026

Mark Tuckerman *Session Chair*

Dong Hui Zhang 08:30–09:10

Water Clusters and Bulk Simulations with an Accurate Universal Potential

Francesco Paesani 09:10–09:50

From Water to Biomolecules: Data-Driven Many-Body Potentials for Predictive Molecular Simulations

Ganglong Cui *Session Chair*

Zhigang Shuai 10:20–11:00

Time-Dependent DMRG for Quantum Dynamics

Daniel Escudero 11:00–11:40

Quantum Chemical and Dynamical Simulations to Unravel Complex Photophysics

Yunlong Xiao *Session Chair*

Trond Saue 14:00–14:40

Quantum Electrodynamics for Chemistry

Christoph van Wüllen 14:40–15:20

Quasi-Relativistic (Two-Component) Hamiltonians

Bingbing Suo *Session Chair*

Garnet Chan 15:50–16:30

Towards Reaction Mechanism Discovery in Biological Systems

Xiaosong Li 16:30–17:10

Breaking the Quadrillion Determinant Barrier in Numerically Exact Configuration Interaction

Eberhard K. U. Gross *Session Chair*

Poster Session 17:10–18:00



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Xiao Lun Auditorium (C101), CCME



Wednesday, July 29, 2026

Chen Li *Session Chair*

Frank Neese 08:30–09:10

New Developments in the Quantum Chemistry of Open Shell Systems

Wenjian Liu 09:10–09:50

Size-Extensive General-Model-Space Many-Body Theories

Hui Li *Session Chair*

Eli Pollak 10:20–11:00

The Semiclassical Route to Ab Initio Quantum Dynamics

Nandini Ananth 11:00–11:40

Excited State Charge and Energy Transfer Mechanisms from Modern Semiclassical Theory

William Glover *Session Chair*

Michele Ceotto 14:00–14:40

Non-adiabatic Semiclassical Molecular Dynamics

Fabien Gatti 14:40–15:20

Quantum Dynamics with the Multi-Configuration Time-Dependent Hartree (MCTDH) Method

Elise Dumont *Session Chair*

Basile Curchod 15:50–16:30

Describing Photoexcitation in Nonadiabatic Molecular Dynamics

Eberhard K. U. Gross 16:30–17:10

The Exact Factorization, A Universal Approach to Non-Adiabaticity