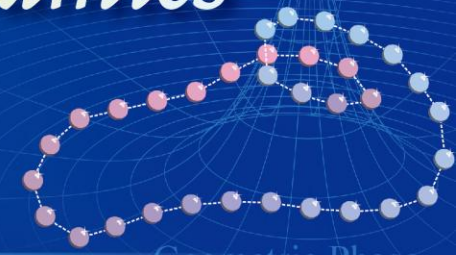
AIQMD2026

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	Sorbonne Univ.	**Seogjoo J. Jang**	City Univ. New York	**Eli Pollak**	Weizmann Institute
Nandini Ananth	Cornell Univ.	**Leeor Kronik**	Weizmann Institute	**Trond Saue**	CNRS / UT3 Paul Sabatier
Victor Batista	Yale Univ.	**Zhenggang Lan**	South China Normal Univ.	**Andreas Savin**	CNRS / Sorbonne Univ.
Jianshu Cao	MIT	**Shuhua Li**	Nanjing Univ.	**Matthias Scheffler**	NOMAD Laboratory
Tucker Carrington	Queen's Univ.	**Xiaosong Li**	Univ. Washington	**Dmitry Shalashilin**	Univ. Leeds
Michele Ceotto	Univ. Milan	**Wenjian Liu**	Shandong Univ.	**Zhigang Shuai**	CUHK-Shenzhen
Rachel Crespo Otero	Univ. College London	**Nancy Makri**	UIUC	**Seiichiro Ten-no**	Kobe Univ.
Basile Curchod	Univ. Bristol	**Reinhard Maurer**	Univ. Wien	**Mark Tuckerman**	New York Univ.
Garnet Chan	CalTech	**Akira Nakayama**	Univ. Tokyo	**Christoph van Wüllen**	TU Kaiserslautern
Weinan E	Peking Univ.	**Frank Neese**	MPI Kohlenforschung	**Xin Xu**	Fudan Univ.
Jiali Gao	Univ. Minnesota	**Francesco Paesani**	UCSD	**Weitao Yang**	Duke Univ.
Fabien Gatti	CNRS/Univ. Bourgogne Europe	**Piotr Piecuch**	Michigan State Univ.	**Dong Hui Zhang**	DICP, CAS

Sponsors:

太一量生 ByteDance fieldQuantum 量坤科技 DP Technology 深势科技 PARATERA 并行 XtalPi 晶泰科技 Chinese Journal of Chemical Physics ACS Publications QUANTUM CHEMISTRY ΨQMD

Summer School: Frontiers in Ab Initio Quantum Molecular Dynamics

Xiao Lun Auditorium (C101), CCME

Saturday, July 25, 2026

Weihai Fang *Session Chair*

Nancy Makri *08:30–09:10*

Numerically Exact Real-Time Path Integral Methods for Quantum Dynamics

Victor Batista *09:10–09:50*

Quantum Machine Learning in Chemistry

Jiushu Shao *Session Chair*

Jianshu Cao *10:20–11:00*

Polariton Chemistry: Quantum Control with Cavity Photons

Dmitry Shalashilin *11:00–11:40*

Electrophore Model for Dissociation of Molecules After Electron Impact in Plasma

Wenjian Liu *Session Chair*

Weinan E *13:30–14:10*

Large atomistic models: from DPA-1 to DPA-4

Mark Tuckerman *14:10–14:50*

From Quantum Statistics to Dynamics: Machine learning and other algorithms for quantum simulation via path integrals

Xiaodong Wen *Session Chair*

Xin Xu *15:20–16:00*

Efficient Pair-Density Functional Theory for Complex Molecular Systems

Andreas Savin *16:00–16:40*

Correction of the Basis Set Error Due to the Absence of the Electron-Electron Cusp in the Wave Function by Using an Adiabatic Correction

Basile Curchod *Session Chair*

Hands-on Activities *17:00–18:00*

Summer School: Frontiers in Ab Initio Quantum Molecular Dynamics

Xiao Lun Auditorium (C101), CCME

Sunday, July 26, 2026

Hong Jiang *Session Chair*

Matthias Scheffler *08:30–09:10*

Interpretable AI with Quantified Trust for the Discovery of Energy Materials

Reinhard Maurer *09:10–09:50*

Ultrafast Dynamics at Surfaces with Machine Learning Surrogates

Wei Hu *Session Chair*

Shuhua Li *10:20–11:00*

Equation-of-motion Block-correlated Coupled Cluster Methods as Electronic Structure Drivers for Nonadiabatic Dynamics Simulations

Seiichiro Ten-no *11:00–11:40*

Recent Advances of Projective Transcorrelation Theory

Haobin Wang *Session Chair*

Tucker Carrington *13:30–14:10*

Using a product contracted basis and optimised collocation points to solve the Schroedinger equation

Rachel Crespo-Otero *14:10–14:50*

Understanding excited state processes in molecular crystals

Jiali Gao *Session Chair*

Hands-on Activities *15:20–16:40*

Reinhard Maurer *Session Chair*

Hands-on Activities *17:00–18:00*

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

Andrey Vasenko *Session Chair*

Piotr Piecuch *13:30–14:10*

H_3^+ Formation from Methyl Halogens and Pseudohalogens: Experiment, Theory, and Governing Factors

Federica Agostini *14:10–14:50*

Theory and Simulations of Ultrafast Processes in Molecules

Xuefei Xu *Session Chair*

Seogjoo J. Jang *15:20–16:00*

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

Akira Nakayama *16:00–16:40*

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

Daniel Escudero *Session Chair*

Hands-on Activities *17:00–18:00*

Summer School: Frontiers in Ab Initio Quantum Molecular Dynamics

Xiao Lun Auditorium (C101), CCME

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 *13:30–14:10*

Quantum Electrodynamics for Chemistry

Christoph van Wüllen *14:10–14:50*

Quasi-Relativistic (Two-Component) Hamiltonians

Bingbing Suo *Session Chair*

Garnet Chan *15:20–16:00*

Towards Reaction Mechanism Discovery in Biological Systems

Xiaosong Li *16:00–16:40*

Breaking the Quadrillion Determinant Barrier in Numerically Exact Configuration Interaction

Eberhard K. U. Gross *Session Chair*

Poster Session *16:40–18:00*

Summer School: Frontiers in Ab Initio Quantum Molecular Dynamics

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 *13:30–14:10*

Non-adiabatic Semiclassical Molecular Dynamics

Fabien Gatti *14:10–14:50*

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

Elise Dumont *Session Chair*

Basile Curchod *15:20–16:00*

Describing Photoexcitation in Nonadiabatic Molecular Dynamics

Eberhard K. U. Gross *16:00–16:40*

The Exact Factorization, A Universal Approach to Non-Adiabaticity