

OpenMolcas Developers' Workshop 2026

14th edition · Scientific Programme

Instituto de Ciencia Molecular (ICMol) · Universitat de València

■ Keynote ■ Oral communication ■ Flash communication ■ Break / social

Monday

REGISTRATION

INTRODUCTION AND TRIBUTE TO LUIS SERRANO ANDRÉS

10:00–10:30

KEYNOTE

OpenMolcas after COVID-19

Ignacio Fernández-Galván · TU Dortmund University, Germany

10:30–10:50

ORAL

CI Algorithms in OpenMolcas

Roland Lindh · Uppsala University, Sweden

10:50–10:55

FLASH

Flash Oral Communication

10:55–11:00

FLASH

Flash Oral Communication

COFFEE

11:30–12:00

KEYNOTE

Multireference Wave Functions in Polarizable Solvent Environments: The Fluctuating-Charge Approach

Chiara Cappelli · Scuola Normale Superiore, Pisa, Italy

12:00–12:20

ORAL

Tuning photochemistry with static electric fields

Nicolas Ferré · Aix-Marseille Université, France

12:20–12:40

ORAL

Photodynamics of Multi-Mode Multi-State Molecular Quantum Systems in a Dissipative Environment

David Picconi · Heinrich Heine University Düsseldorf, Germany

12:40–12:45

FLASH

Flash Oral Communication

12:45–12:50

FLASH

Flash Oral Communication

12:50–12:55

FLASH

Flash Oral Communication

12:55–13:00	FLASH Flash Oral Communication
	LUNCH
15:00–15:20	ORAL Hybrid QM/MM NAMD simulations Igor Schapiro · TU Dortmund University, Germany
15:20–15:40	ORAL Light-Activated Mechanisms in DNA: the Origin of Multiple Rare Mutations? Irene Conti · Università di Bologna, Italy
15:40–16:00	ORAL Nonadiabatic Molecular Dynamics under External Forces in OpenMolcas Luis Manuel Frutos · Universidad de Alcalá, Spain
16:00–16:05	FLASH Flash Oral Communication
16:05–16:10	FLASH Flash Oral Communication
16:10–16:15	FLASH Flash Oral Communication
16:15–16:20	FLASH Flash Oral Communication
16:20–16:25	FLASH Flash Oral Communication
	POSTER + REFRESHMENTS

Tuesday

09:30–10:00

KEYNOTE

From Multiconfigurational Wave Functions to Single/Oligo-CSF Descriptions: The Quantum Anamorphosis

Giovanni Li Manni · Max Planck Institute for Solid State Research, Stuttgart, Germany

10:00–10:20

ORAL

Electron correlation: The roads less traveled by

Francesco Aquilante · EPFL, Switzerland

10:20–10:40

ORAL

Extending Automated Selection of Nuclear Coordinates for Reduced Dimensionality Non-adiabatic Dynamics: Sparse PCA and Alternative Coordinate Systems

Alessandro Nardi · Nantes Université, CNRS, CEISAM, France

10:40–11:00

ORAL

Density Matrix Renormalization Group to target Core Excited States of Transition Metal Complexes

Giacomo Bassi · Technical University of Munich

COFFEE

11:30–12:00

KEYNOTE

Three Views on Nonadiabatic Dynamics

Sandra Gómez · Universidad Autónoma de Madrid, Spain

12:00–12:20

ORAL

An Ultrafast Dynamics Kaleidoscope with OpenMolcas

Sergey Bokarev · Technical University of Munich, Germany

12:20–12:40

ORAL

Anharmonic Vibronic Coupling Model in Trajectory Surface Hopping Simulations at the MS-CASPT2 level of theory

Jesús Lucia-Tamudo · University of Vienna, Austria

12:40–13:00

ORAL

One, Two, Three Irons: From Multireference Photochemistry to Magnetic Frustration

Leticia González · University of Vienna, Austria

LUNCH

TOUR · CIUTAT DE LES ARTS I LES CIÈNCIES

Wednesday

09:30–10:00

KEYNOTE

OPAL – Orbitals, Plotting, Analysis, and Layout

Luca de Vico · Università di Siena, Italy

10:00–10:20

ORAL

Vibrationally Resolved Spectroscopy at Multireference Perturbative Level: An OpenMolcas–FCClasses3 Interface

Javier Cerezo · Universidad de Murcia, Spain

10:20–10:40

ORAL

Can we describe electron charge Transfer in Magnetite in embedded cluster calculations

Marek Krośnicki · University of Gdańsk, Poland

10:40–11:00

ORAL

DRAGON@OpenMolcas: A New Interface for Diabatization of Excited States in Molecular Aggregates

Jesús Cerdá · Universitat de València – Instituto de Ciencia Molecular (ICMol), Spain

COFFEE

11:30–12:00

KEYNOTE

From Quantum Algorithms to Better Therapies and Materials: Transitioning from Near-Term to Early Fault-Tolerant Impact in Quantum Computing for Molecular Simulations

Stefan Knecht · Algorithmiq Ltd, Finland

12:00–12:20

ORAL

Stop Programming? AI Agents for Scientific Software Development

Valera Veryazov · Lund University, Sweden

12:20–12:40

ORAL

First baby steps towards a GPU-based CASSCF-CASPT2 (OpenMolcas ?) software

Marco Garavelli · Università di Bologna, Italy

12:40–13:00

ORAL

GronOR, a massively parallel and GPU-accelerated code for non-orthogonal configuration interaction

Coen de Graaf · Universitat Rovira i Virgili, Spain

LUNCH

ROUND TABLE

CLOSING AND AWARD CEREMONY