



COST Action CA18212

MD-GAS

Molecular Dynamics
in the GAS phase



Visit GdańskTech!

MD-GAS TRAINING SCHOOL

**Theory and modelling of
dynamics of molecules and
clusters in the gas phase**

3-7 JULY 2023

**GDAŃSK UNIVERSITY OF
TECHNOLOGY, POLAND**

Learn from leaders in
science

About MD-GAS

The main aim of the MD-GAS COST Action (CA18212) is to develop a new physical and chemical toolbox to significantly advance the understanding of:

- gas phase molecular dynamics induced in interactions between molecules or clusters and photons, electrons, or heavy particles;
- its consequences for a broad range of applications in e.g. astrochemical and atmospheric sciences, and molecular radiation damage.

About the school

The participation at the school is free of charge. The training school will cover a broad range of topics in the theory of molecular dynamics as well as application and development of theoretical tools, which provide new opportunities in molecular physics and physical chemistry. The school will be held on-site with attendance limited to 55 trainees and with priority given to PhD students and early career researchers, which are warmly invited to participate. Lectures given by experts in the related fields will be coupled with "hands on" tutorials organized at the computer labs of Gdańsk Tech. Every participant is expected to present a poster about their research.

Registration and more info at:

<https://ftims.pg.edu.pl/en>



school2023@mdgas.eu
<https://mdgas.eu/>





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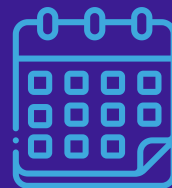
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FACULTY OF APPLIED
PHYSICS AND MATHEMATICS



**REGISTRATION
DEADLINE
JUNE 18TH**



Registration and financial support

The MD-GAS COST Action will provide financial support for a limited number of Early Career Researchers. The participants interested in the support can submit an application during registration before **June 2nd**.

Final registration deadline is **June 18th**.

Location

The school will take place at the Faculty of Applied Physics and Mathematics of Gdańsk University of Technology. Gdańsk is easily accessible by all means of transport. The most convenient way to get to the city is to fly to the Gdansk Lech Wałęsa Airport that is located 10 km away from the center of Gdańsk. You may also travel to Warsaw Frederic Chopin Airport, or Warsaw Modlin Airport, situated about 350 km from Gdańsk, and reach your final destination by train or by bus.

Accommodation and meals

The attendees are expected to arrange their own accommodation. Gdańsk is a very popular tourist destination, especially during the summer, so please make sure you book your stay in advance. Cheap accommodation in walking distance from the university campus can be booked at the [student dormitory](#).

Lunches will be served by an external company (approx. EUR 15-20 per lunch). Payment details will be sent to interested participants after registration.

Activities

Apart from lectures and tutorials participants will have an opportunity to visit the local supercomputer centre at the new facility of the Centre of Informatics Tricity Academic Supercomputer and networkK (CI TASK) as well as present their research at a poster session.

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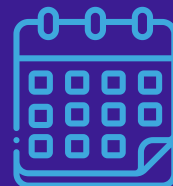


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Tutors and program



César Mogo

Universidade do Algarve, Portugal

*From atoms and molecules to complex reaction systems
simulations: The MreaDy approach*



Emilio Martinez-Nuñez

Universidade de Santiago de Compostela, Spain

Automated Reaction Discovery using MD Simulations



Sergio Díaz-Tendero

Universidad Autónoma de Madrid, Spain

*Dynamics of ionized molecules and molecular clusters in the
gas phase*

Jesús González-Vázquez

Universidad Autónoma de Madrid, Spain

*Semiclassical dynamics on electronic excited states using
surface hopping*



Eva Muchova

University of Chemistry and Technology, Prague, Czechia

*Highly excited and ionized states and follow-up ultrafast
processes*



Aude Simon

Université Paul Sabatier, France

*Molecular dynamics of large molecules and clusters using
the DFTB method*



Local Organizers : Marta Łabuda, Ewa Erdmann

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