032CM - 2026

PROGRAMMING FOR COMPUTATIONAL CHEMISTRY

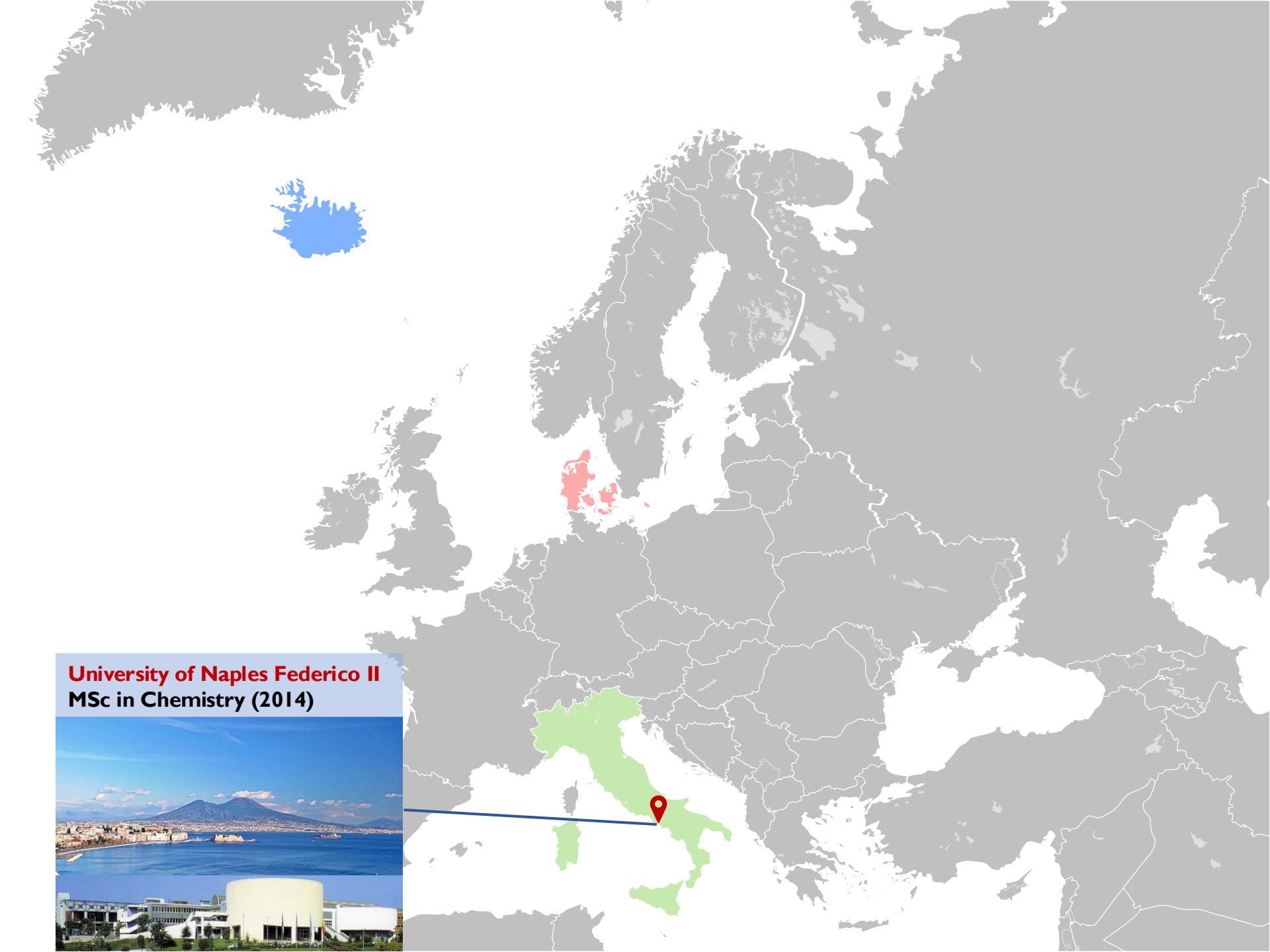
Presentations

Gianluca Levi

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Office: Building C11, 3rd floor, Room 329

Fall 2026


University of Naples Federico II
MSc in Chemistry (2014)

Technical University of Denmark
PhD in Theoretical Physical Chemistry (2018)





University of Naples Federico II
MSc in Chemistry (2014)







University of Iceland
Postdoc (2018 - 2024)
Research Specialist (2025 -)

Technical University of Denmark
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PhD in Theoretical Physical Chemistry (2018)
University of Naples Federico II
MSc in Chemistry (2014)
University of Trieste
Assoc. Professor (2025 -)

What I teach

Courses for graduate and undergraduate students in chemistry, biochemistry and chemical engineering

2025 - present **Programming for computational chemistry**

University of Trieste

2022 - present **Molecular Spectroscopy and Reaction Dynamics**

Computational Chemistry

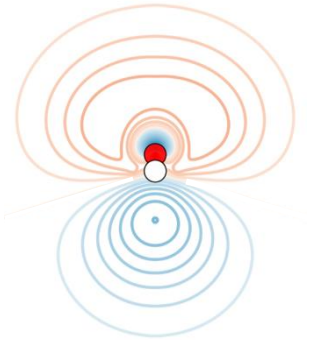
University of Iceland

My research activities

What happens when molecules absorb light?

Method development

Electronic structure methods and software for modelling **excited states**, multiscale methods for **molecular dynamics**



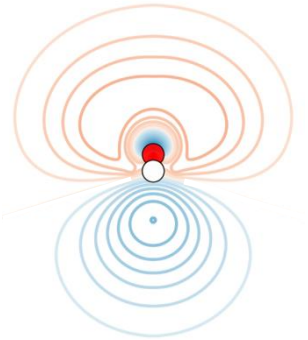
$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = \hat{H}(t)\left|\Psi(t)\right\rangle$$

$$\ddot{\mathbf{R}}_\alpha = -\frac{\nabla_\alpha E_i}{M_\alpha}$$

https://gialev.github.io/

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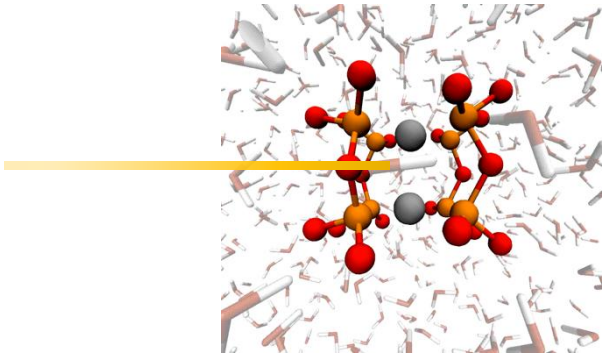


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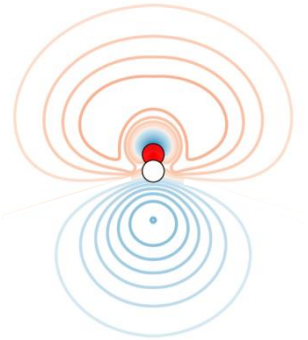
Simulations

Excited states, charge transfer, and atomic motion in systems relevant to **solar energy conversion**, **photocatalysis**, and **astrochemistry**

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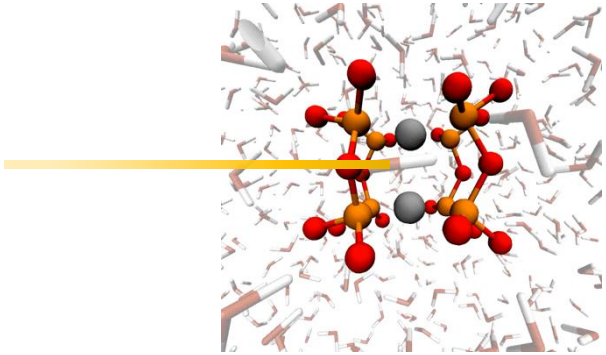


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Observations

Time-resolved experiments at large-scale facilities to track light-induced molecular dynamics in solution





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